Fresenius J Anal Chem (1992) 343:827–828

Fresenius' Journal of Analytical Chemistry

Analytical Chemistry – today's definition and interpretation

K. Danzer

Friedrich-Schiller-Universität Jena, Chemische Fakultät, Lehrstuhl Analytik, Steiger 3, O-6900 Jena, Federal Republic of Germany

Received February 6, 1992

Introduction

Analytical Chemistry has developed in the past decades into an independent chemical discipline with a multidisciplinary nature [1–6]. This has resulted in the need for a topical definition and interpretation of Analytical Chemistry which takes into account the complex nature of its aims, objects, and methods as well as their correlations.

It seems that Analytical Chemistry is again at a crossroad in its development. After universality in the 19th century [7], Analytical Chemistry was pushed into the role of a kitchen-maid at the turn of the century [8]. In the past 40 to 50 years a rapid instrumental evolution occurred, connected with considerable progress in microelectronics and computers, to realize the growing demands of qualitative and quantitative materials chemistry, environmental research, clinical chemistry, toxicology, biotechnology, and microelectronics.

This development includes the danger that Analytical Chemistry may become a measuring slave for other chemical and non-chemical disciplines being confined by regulations and choked under a flood of data. In reality, Analytical Chemistry has disclosed new dimensions of its aims, objects, and methods in an interdisciplinary way which requires an up-to-date definiton of Analytical Chemistry.

Definition

The object of Analytical Chemistry is to obtain chemical information about materials concerning their qualitative and quantitative composition and structure. Analytical Chemistry investigates the type and the quantity of components and the structural relations between the constituents. Analytical investigations are directed to solve general problems and, for this purpose, to develop and to advance analytical methods including sampling, sample preparation, and evaluation, and to apply statistics and data analysis for the interpretation of analytical results.

Interpretation

The subject of Analytical Chemistry can be summarized in the scheme of the analytical process (Fig. 1). The analytical process gives an account of the general action for all analytical investigations independent of whether they deal with identification and determination of components or structural elucidation.

In each case it is important that the three parts of all analytical investigations: the problem, the sample and the method used, comply with each other in an optimum way (Fig. 2).

The representativeness of the sample plays a particular role within this circle. A sample must be representative in three ways: (1) concerning the object, especially its homogeneity or heterogeneity and its quantity, (2) concerning the analytical problems, e.g. if an average analysis, a local or distribution analysis is required, and (3) concerning the special demands of the method for which the sample must be prepared.

Analytical methods are the fundamental tools of the analyst. They are based on chemical reactions and electrochemical processes as well as on interactions with all forms of energy, particularly radiation. Although most of the methods are based on physical principles, the connection to chemistry is given through the material aspects of the sample and by the need for chemical calibration or certification. Figure 3 shows a systematic outline of essential analytical measurement principles.

For modern analytical measurements, coupling of several methods and techniques are characteristic. This concerns separation and enrichment techniques coupled with methods of determination (gas-chromatography/mass spectrometry, flow injection/solid phase extraction /atomic absorption spectrometry) as well as several techniques of analysis to increase the efficiency of such single steps as ablation, atomisation, excitation, and detection (laser ablation/inductively coupled plasma spectrometry/mass spectrometry). In this way a various interlacing of methods takes place without

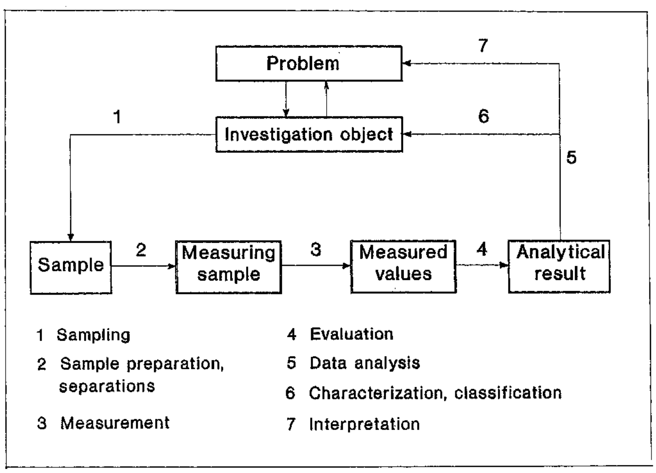

Fig. 1. The analytical process [6]

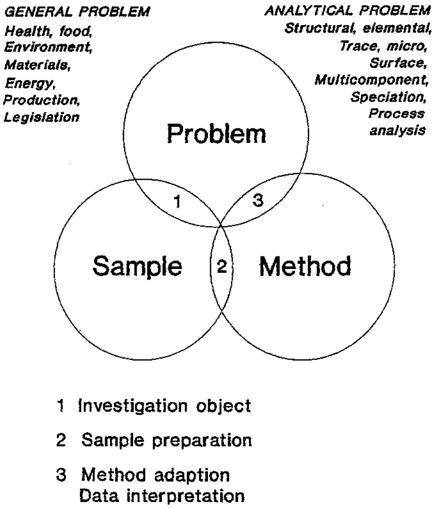

Fig. 2. The unity of the three parts of analytical investigations

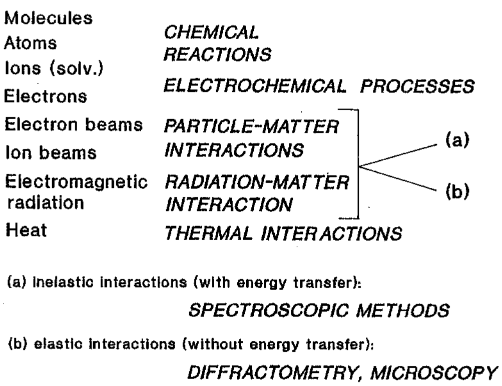

Fig. 3. Interactions of matter and energy with samples

loss of independence of each method, so that the variety of analytical methods and combinations permanently increases.

Analytical Chemistry has to be handled in the trinity of problem, sample, and method as the science which solves general problems by extraction of information about samples by means of analytical methods.

From the chemical point of view, Analytical Chemistry deals with the identification and determination of chemical elements and compounds which may occur in the form of atoms, ions, molecules, or crystals. In the latter case structural relations may be investigated in a qualitative or quantitative way. As it is usual to distinguish between qualitative, semi-quantitative, and quantitative elemental analysis, it may be useful to call these:

– qualitative structural analysis in the case of structural elucidation as demonstrated by graphic molecular formulae, crystal type, or space lattice type.

– semi-quantitative structural analysis in case of characterization of steric isomers, and

– quantitative structural analysis if spatial parameters like atomic distances and angles in molecules or lattice spacings and angles in crystals are to be determined.

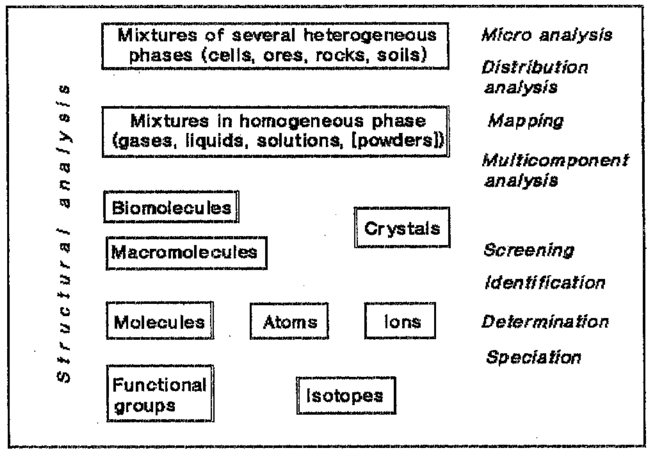

Fig. 4. Extent of analytical investigations (derived from [5])

The extent of samples studied includes single atoms and isotopes as well as functional groups, molecules, macro- and biomolecules, and mixtures of inorganic and organic matter of complex nature (Fig. 4).

Today, chemometric principles and computer applications are included at all steps of the analytical process, e.g. sampling theory, experimental design, optimization of analytical measurement and separation procedures, calibration, signal processing for improvement of signal-noise ratio and signal resolution, multivariate statistics and data analysis for extraction of useful information from large (multidimensional) data sets, up to intelligent laboratory systems and robotics.

Since the obtaining of information is the object of Analytical Chemistry, analytical results and methods may be characterized also by means of information theory [9–12].

References

1. EUROANALYSIS VII, Vienna (1990) 21st Meeting of WPAC: Education in Analytical Chemistry 1989/90. Recommendations for the Future by WPAC of FECS
2. Mottola HA (1991) Anal Chim Acta 242:1–3
3. Murray RW (1991) Anal Chem 63:271A
4. Tyson JF (1988) Anal Proc 25:111–114
5. Kelker H, Kraft G, König K-W (1980) Aufgaben und Methodik analytischer Verfahren, Ullmanns Encyklopädie der technischen Chemie, 4. Aufl Bd 5: Analysen- und Meßverfahren. Verlag Chemie, Weinheim, pp 1–25
6. Danzer K, Than E, Molch D, Küchler L (1987) Analytik – Systematischer Überblick. Akadem Verlagsges, Leipzig, Wiss Verlagsges, Stuttgart (2. Aufl)
7. Kelker H (1988) Mitt-bl Fachgr Anal Chem GDCh 55:M185–187
8. Ostwald W (1894) Die wissenschaftlichen Grundlagen der analytischen Chemie. Verlag W. Engelmann, Leipzig, S V
9. Eckschlager K, Stepanek V (1979) Information theory as applied to chemical analysis. Wiley, New York
10. Danzer K, Eckschlager K, Wienke D (1987) Fresenius Z Anal Chem 327:312
11. Danzer K, Eckschlager K, Matherny M (1989) Fresenius Z Anal Chem 334:1
12. Danzer K, Schubert M, Liebich V (1991) Fresenius J Anal Chem 341:511