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Analytical chemistry and chemical analysis

Analytical chemistry is often identified with chemical analysis. Nevertheless, the relationship between the analytical chemistry and chemical analysis is much the same as that between medical science and medical practice.

Modern analytical chemistry can be defined as a science concerned with the development of general approaches, methods and tools for the study of chemical compositions of substances and analysis of objects; chemical analysis is restricted to acquisition of information about chemical compositions of substances.

Chemical analysis is an essential tool for qualitative estimation of miscellaneous products and control over environmental objects and technological processes; besides, it is a valuable diagnostic tool in medicine. It is used in routine criminalistic studies and military practice. The conclusions in many sciences, such as molecular biology, geochemistry, chemical kinetics, *etc*., are based, to a great extent, on the results of chemical analysis.

On the global scale, the number of analyses can be indirectly estimated, if one recalls at least some wide spread analyses, *e.g*., measurements of carbon, phosphorus and sulfur in melted steels; of aromatic hydrocarbons and sulfur in natural oils and petroleum products; of carbon monoxide and hydrocarbons in motor car exhausts; of chlorine in swimming pool water; of pH levels in soils; of moisture content in grains and of fat content in milk, and, finally, analyses of blood and urine samples in clinical laboratories.

The range and complexity of problems facing chemical analysis and, as a consequence, analytical chemistry as a science, are steadily increasing with an increase in the number of subjects to be analysed. Who, in the middle of the 20th century, might surmise that the objects for investigation in molecular biology, biochemistry, biotechnology and, perhaps, contemporary medicine would occupy an important place among objects for analytical investigations; that the necessity of analysing complex oxides would emerge in connection with the discovery, in the 1980's, of high-temperature superconductivity; that rapid development of electronic engineering would place high-purity elements into the group of most important and most difficult objects of chemical analysis?

The number of problems facing chemical analysis and control over 'classical' objects and the new ones that constantly appear is also increasing. One of them, related to the increase in the number of components to be identified and characterised, demanded novel analytical methods for its solution. Thus inductively coupled plasma atomic emission spectroscopy (ICP-AES) made simultaneous measurement of 30 – 40 elements a routine practice, while the use of ICP-mass spectrometry made possible simultaneous determination of 60 elements at a sufficiently high level of sensitivity. Gas chromatography on capillary columns enables detection and, to some extent, quantitation of several hundred components of tested objects (*e.g*., over 400 components were identified in coffee aroma). This list is far from being complete, and the problems continue to emerge over and over again.

In recent years, a demand arose for local (distribution) analysis as an alternative to bulk analysis, since in many objects the analysed components are characterised by non-homogeneous or non-uniform distribution over the thickness of the sample. The necessity to solve this task led to the development of complex and expensive instrumental methods, such as electronic probe, X-ray electron and Auger spectroscopy, sophisticated versions of mass spectrometry, *etc*. It can be expected that the range of problems to be solved by distribution analysis will continue to expand in the future.

Problems demanding non-destructive analysis of specimens (*e.g*., material exhibits, archeological finds, medieval paintings, *etc*.) arise regularly in some other fields, *e.g*., technology, criminalistics, archeology, fine arts, science, *etc*., aimed at prolongation of their functioning where required. Today, these problems are solved with either the help of X-ray fluorescence analysis, radioactivation method (in the case of short-lived radioisotopes) and IR spectroscopy or techniques producing minute destruction (electron probes, atomic emission analysis, *etc*.). There is no end to work here, and novel simple and inexpensive original procedures are required.

As time goes on, the need for continuous analysis (*e.g*., on-line downstream analysis of sea water or express analysis of ore on a conveyor belt) as well as remote analysis (*e.g*., control over technological processes involving radioactive or highly toxic substances or examination of extraterrestrial objects) is increasing. This is the scope of spectroscopic and electrochemical methods. However, challenging (or altogether intractable) problems of remote analysis still exist and tomorrow they will be even more numerous.

Throughout its history, analytical chemistry was trying to solve problems connected with increasing the sensitivity, accuracy, selectivity and rapidity of analysis and not without advantage. Today, there is seemingly no need in ultraprecise methods; the level of precision attained is usually very high. However, with consideration that practical requirements are changing continuously, the analysts must be ahead of time while developing ultraprecise methods for analysis.

On the other hand, it is not always necessary to perform multicomponent determinations. Sometimes, it is sufficient to establish a common parameter (the so-called integral index), which represents a cumulative effect of the whole gamut of the components. For instance, natural potable water can contain phenols, which are disagreeable by themselves, but especially hazardous are the toxic organochlorine compounds formed upon chlorination of water with participation of phenols. The detection of diverse phenolic species (nitrophenols, cresols, *etc*.) and, particularly, quantitation of each of them is a labour- and time-consuming process, at the least. However, their presence and total content can be established with the help of a single group reaction that is common for all phenols. This parameter is usually referred to as the 'phenol index' and provides a very simple example of the integral index. The degree of water pollution with oxidisable substances can be established with the help of an integral index called chemical oxygen demand (COD), which is determined from the consumption of an oxidant (as a rule, dichromate) and is proportional to the degree of contamination of water with organic compounds. Other determined parameters include total concentrations of heavy metals and polynuclear aromatic hydrocarbons. If such assays give positive results, individual analyses of compounds have to be performed where necessary.

Screening (two-step analysis) is usually employed in wide spread analyses in order to reduce labour, time and reagent consumption; in its first step, samples containing no components that are looked for are rejected. The negative result (*i.e.*, lack of the component) is considered to be final and the corresponding samples are excluded from subsequent analysis. The 'positive' samples are analysed more carefully. In this approach, the first step may include simplified and relatively inexpensive procedures, *e.g.*, test methods.

The mass character of analyses is provided by unification of experimental procedures. Carefully selected, repeatedly approved, well-developed techniques facilitate test operations. Standardisation is the highest grade of unification: while the use of unified protocols can only be recommended, the use of standardised protocols is often compulsory.

The productivity of analyses can be increased through automation and computerisation of analytical procedures. Thus the number of samples tested in agrochemical laboratories increased sharply after reorientation to analytical conveyors and the so-called continuous flow analysis.

The need for laboratory analyses is reduced with the advent of novel analytical methods and tools for their realisation: the instruments become more compact and portable and the methods are gradually becoming reagent-free as is the case with X-ray fluorescence analysis. Moreover, some analytical investigations, *e.g.*, remote analyses of extraterrestrial objects, cannot either be realisable in principle or impractical under laboratory conditions (*e.g.*, measurements of CO content in motor car exhausts or of methane content in coal mines).

The recently developed chemometric technique is yet another novel approach towards analysis. This area of research is intermediate between chemistry (analytical chemistry, in the first place), mathematics and information theory. For instance, the chemometric approach named image recognition has proved to be efficient in the analysis of complex mixtures. Here, the very paradigm of chemical analysis is changed and we renounce the idea of a 'one-after-another-component analysis'.

Since the middle of the 20th century, classical chemical methods of analysis have been continuously replaced by instrumental methods based on the use of physical phenomena, physicochemical regularities and most recent achievements in electronics, mathematics and informatics as well as in biochemistry, immunology and other biological sciences. Today, the absolute majority of practical analyses are carried out using these methods. Whereas in 1951 gravimetric, titrimetric and colorimetric methods were used as the major analytical procedures for certification of the most popular and universally employed standard geological samples, X-ray fluorescence and mass-spectrometric methods came to the foreground in 2004 – 2005.

The significance and abundance of one or another method change with time and space [*i.e.*, the place (country) where the analysis is carried out]. Its choice relies not only on its analytical potential and practicability for the solution of specific tasks, but also on extraneous (sometimes, critical) circumstances, such as financial situation, availability of experts, working areas, just traditions and even prejudices.

Hybrid methods became especially popular in the past decade; this refers primarily to a combination of separation and measuring techniques, *e.g.*, capillary electrophoresis and virtually all modern chromatographic techniques that combine chromatographic columns with detectors for continuous determinations. Flow-injection analysis is also related to hybrid methods, except that in this case the role of a column is played by a sampling unit, which includes an injector, chemical reactors and often a preconcentration device.

The recent trend is towards miniaturisation of analysis and analytical systems. Generally speaking, the transition from macroanalysis ('wet' chemical analysis) to semimicro- and microanalyses occurred very rapidly in due time; microscopic methods and techniques for ultramicrochemical inorganic analysis and electrochemical analyses of biological objects including isolated cells were devised in the middle of the past century. An attempt to accommodate multifunctional devices on a microelectronic chip is the most promising recent trend; this concerns, in particular, capillary electrophroresis and, to some extent, flow-injection analysis. Many problems remain to be solved, especially in the design of mini-detectors, but the future is more than exciting. Pocket-size mini-analysers for determining a single substance (less frequently, several substances), *e.g.*, gas analysers, already appeared on the market. As a rule, the methodology for their operation is built-in, no calibration is also necessary. The instrument control is very simple: a single touch of a key and the result is displayed on the screen. The first devices of this type were, most probably, pH-metres.

However, an opposite trend, *i.e.*, the design and manufacture of sophisticated multifunctional instruments able to perform not one, but two or several related analytical procedures, also exists. The devices for surface analysis can serve as examples. These bulky and very expensive instruments combine X-ray emission microanalysis (electronic probe) with X-ray (photo)electronic and Auger spectroscopy and even secondary-ion mass spectrometry. It is noteworthy that the commercial production of analytical instruments is among the most dynamically developing branches of industry all over the world.

The formulation of adequate policy with regard to laboratory facilities still presents a problem. In case of difficult financial situations and high production cost of complex, often multifunctional instruments, their collective purchase and maintenance are of vital importance.

In conclusion, let us note once again the main trends in the development of modern analytical chemistry:

— miniaturisation of analysis including development of general-purpose analytical instruments and simple analysers based on microelectronic chips with microfluid and other systems;

— explosive development of methods and tools for extralaboratory ('field') chemical analyses including design of efficient easy-to-use tools for on-site detection of explosives and drugs;

— use of the most recent advances in mathematics and information theory (chemometrics) for effecting the transition from conventional ('one-after-another-component') analyses to estimation of integral indices and image recognition; design of expert systems; design of an 'electronic nose' and an 'electronic tongue'; development of approaches to multiparametric calibration;

— further improvement of methods and tools for distribution (local), continuous (flow-type), remote and non-destructive analyses;

— design of novel, in principle, tools for chemical analysis based on the use of nanotechnologies including development of continuously operating chemical sensors;

— expansion of studies aimed at perfection of analyses of biomedical objects;

— search for novel principles of generation of analytical signals, *e.g.*, the use of solid chemical (semiconductor, acoustic, *etc.*) sensors;

— further development and improvement of the existing spectroscopic, mass-spectrometric, chromatographic, electrochemical, *etc.* methods of analysis including surface analyses.

The past decade was marked by a departure from the conventional term 'analytical chemistry' to the term 'analytics'. This tendency is not random, of course. The matter of analytical chemistry underwent significant transformations. Today, it is far from being a mere chemistry, but rather an interdisciplinary science, which belongs partly to chemistry and partly to physics. To a considerable degree, the science of chemical analysis rests upon mathematics, information theory and biological sciences. Among analysts (especially those who are concerned with spectroscopic and nuclear-physical methods of analysis), physicists and engineers constitute rather a large group. They are analysts, but not chemists.

The present issue of the *Russian Chemical Reviews* is devoted to the state-of-the-art in individual methods of chemical analysis, since the description of all existing procedures cannot be published in one issue. Chemometric problems are considered in the review by O Ye Rodionova and A L Pomerantsev 'Chemometrics: achievements and prospects'. Spectrometric methods of analysis are described in the reviews by A A Bol'shakov *et al*. 'Prospects in analytical atomic spectrometry' and by A Kh Gilmutdinov *et al*. 'Spatially resolved atomic absorption spectrometry'. The prospects for Mössbauer spectroscopy in chemical analysis are discussed in the review by V G Semenov *et al*. The review by Ya I Yashin and A Ya Yashin 'Analytical chromatography. Methods, instrumentation and applications' is devoted to the state-of-the-art in chromatographic methods of analysis. And, finally, the review by S B Savvin *et al*. deals with the description of various methods for modification of organic reagents used in spectrophotometric assays.

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