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FEATURE ARTICLES

On the Methodology of Creation of Novel Techniques for Quantitative Chemical Analysis

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Abstract—Sources of new analytical techniques, mainly quantitative, are considered. The birth of novel techniques of quantitative analysis is usually associated with the finding and use of characteristics (properties) of an object, specifically related to the component concentration. The success of such a search substantially depends on the possibility of monitoring advances in many branches of science and instrumentation and of their assessment from the viewpoint of suitability and prospects for analysis.

Keywords: techniques of quantitative analysis, history of methods of analytical chemistry, general scheme of the development of methods of analysis

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Sources of techniques of quantitative chemical analysis and general methodology of their development were considered in several works [1–4]. Thus, a distinction in the schemes of creation of classical and instrumental methods was revealed in monograph [3].

The general principle of techniques of quantitative chemical analysis is based on a dependence of any physical characteristic (property) of an object on the concentration of one or several components, provided a correlation between the concentration and the magnitude of the property exists. The value of the characteristic (analytical signal) must be measured rather easily. For example, in the photometric determination of the concentration of potassium permanganate in solution, the measured characteristic is the absorbance of the solution and the correlation equation is the Bouguer–Lambert–Beer law.

Within this approach, a key factor for the creation of a new technique of quantitative analysis is the finding of characteristics (properties), whose values depend on composition in a definite way. It is clear that the best known, "surface" characteristics (properties) have already been used for a long time. The search for new properties is governed by the scopes and researcher's intuition; it requires creativity. The properties can be found in neighboring fields of science, and often not the next neighbors. The properties can be found incidentally, sometimes in conducting "not analytical" research, as it happened with Heyrovsky, who studied physical and chemical processes on a mercury drop. The application of semiconductor gas sensors, diode lasers, surface ionization, or the degree of extinction of water fleas in polluted water can provide examples of the analytical use of achievements in branches of science quite distant from analytical chemistry. The task of an analyst researcher in this case consists in the careful monitoring of the appearance of essentially new ideas in other branches of science and equipment and their assessment from the viewpoint of their possible use in chemical analysis.

Of course, "neighbors" (physicists, biologists, etc.) in themselves quite often realize analytical possibilities of the new phenomena, regularities and properties they find and devices they develop and even demonstrate these possibilities. In this case, the prompt attraction of professional analysts is important for solving problems about which neighbors have no or lax ideas (interferences and methods of their elimination, principles of calibration, analytical range, resources of materials and devices, reproducibility of the results and metrology in general, etc.). There is a long distance from an observation of a materials scientist about, e.g., the dependence of the resistance of any new substance on the concentration of a particular gas to the creation of a method for the determination of this gas and, more, to the development of a reliable gas analyzer. Moreover, it is not necessarily true that an analytical method itself will be developed.

However, the dependence of a property on the concentration of a component is in some cases highly demanded, particularly in the design of detectors recording changes in the properties of a phase moving in a flow, for example, in capillary electrophoresis or gas chromatography. In this case, one can (which is even better) use a not selective property, characteristic for the whole range of components, for example, heat conductivity or possibility of ionization in a flame.

Amplification, multiplication, and "decontamination" of the value of an already known property is also a very important and most actively used approach. Thus, absorbances in the determination of metal ions are controlled by selecting sensitive and selective reagents; background correction and the use of modifiers provided considerable advances in atomic absorption spectrometry. It is clear that this approach is pragmatically much more important than the search for essentially new properties. Much success can be achieved in this way.

The arsenal of methods of chemical analysis is, certainly, not limited by methods of quantitative analysis. Methods of detection (presence of components), identification of substances, separation, and sample preparation in general, etc. are also of great importance. The invention of, for example, chromatography as a separation method (even before its transformation into a hybrid method, i.e., before the appearance of detectors) was a great achievement.

Analysts themselves can and must find new regularities, phenomena, properties, and approaches to a possible creation of original methods. This was ever done and is done by the most advanced analysts. Examples can be provided by the creation gas chromatography—mass spectrometry by F.W. McLafferty, electrothermal atomic absorption spectrometry by B.V. L'vov, use of Fourier transformation or inductively coupled plasma in spectrometry, electrospray in mass spectrometry, or total external reflection in X-ray fluorescence analysis.

The previously discussed [4] issue about who exactly or, more precisely, what group of researchers created new analytical techniques also adjoins the problem under discussion. Three categories of inventors were distinguished: (1) professional analysts (McLafferty, L'vov); (2) researchers from other sciences coming across phenomena, regularities, or properties that can be used for analysis during their "not analytical" studies (Heyrovsky, laser physicists, materials scientists); and (3) researchers from other sciences who met a need in new tools for solving their professional problems (biochemists invented gel permeation chromatography; Nobel Prizes in recent years have been awarded for numerous similar works).

The general scheme of the creation of a new technique of quantitative analysis can look, for example, as follows [4, 5] (we speak more about logical than chronological sequence of stages). Finding of a suitable characteristic (property)[1]; study or adoption of a functional dependence, expressing a quantitative relationship between the concentration of a component and the value of a property. Creation of a technical device for recording the property value (analytical signal). Development of procedures implementing the technique, elimination of interferences from other components not interesting for the analyst. Evaluation of performance characteristics of the methods based on that technique, reproducibility and accuracy of the results, and limits of determination (concentration and the amount of substance). Assessment of the range of samples to which the analytical technique can be applied (and for which its application is most rational). Comprehensive study of the nature and mechanisms of phenomena and processes on which the technique is based, simultaneously of after a certain time.

[1] To the point, analytical chemistry is sometimes defined as a science dealing with characteristic properties of substances, reflecting their chemical compositions (L.N. Moskvin).

Speaking about the needs arose in "neighbors" (biochemists, geochemists, etc.), we touched upon the subject of motivation. Motivation may be different in different groups of technique inventors. If the neighbors have, first of all, purely applied interests, the same motives in professional analysts quite often move forward fundamental science, curiosity, pursuance of new knowledge in itself, etc. We know examples when new techniques were created long before a need in them appeared; sometimes the author of a technique did not understand its potentials and importance. However, these cases are seldom; professional analysts most often develop new techniques purposefully and consciously.

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