

Trends of analytical chemistry*

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The further development of a specialized branch of science is significantly defined by its own past, with the extension of those social demands which it has to satisfy. Just therefore I would like to give at the beginning of my lecture a survey on the historical antecedents of analytical chemistry.

Historical antecedents

In the history of science the subsequent and parallel application of analysis and synthesis can often be observed in many domains. Within the history of chemistry, since we stepped over from the age of alchemy into the modern period of science, the importance of analysis became predominant. Therefore it was not accidental that in the 18th and 19th centuries analytical chemistry played a fundamental role within chemistry. It is easily understandable also that at the first European technical Academy, founded in Hungary at Selmechánya, the first practical subject was analytical chemistry in the frame of which the blow pipe probe, and other material testing methods were taught.

If we examine the past of analytical chemistry in the period before the Second World War, when those measuring techniques were elaborated and developed which we call already classical, then our attention may be drawn fundamentally to three main trends. In this period gravimetry and its further development played a great role. In the related research there were several trends. Defining the optimum conditions for the precipitation was the goal of this period. We may perhaps say that the final accomplishment of this research trend is characterized by electrogravimetry and thermogravimetry. In the development of the methods it was often characteristic that they were based on empirical results and the explanations seemed often to be speculative. I think we are not far from the truth if we attribute the rather long-lasting decline in the professional appreciation of analytical

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chemistry to this empirical period. Although many good methods were developed in this period, to these methods may the false opinion be attributed, that analytical chemistry is based on the knowledge of kitchen receipts.

The second trend served already as basis to the development of instrumental techniques and was based first of all upon electrochemical experience but applied flame emission and light absorption, too, to the development of analytical methods.

Initiated by the fundamental activity of *Nernst* and the work of *Kohlrausch* electroanalytical methods began to develop. This trend culminated in the activity and results of *Heyrovský*.

Spectrochemical emission analysis especially flame photometry based on the results of *Kirchhoff* and *Bunsen* of the last century was elaborated, but due to the empirical way of its application was not of great efficiency and gave not well reproducible results. In the thirties, first of all due to the activity of *Kaiser* and coworkers, spectrography began its flourishing career, applied mainly in industry to metal and rock analyses.

The analytical application of light absorption was far more extended in practice than the other instrumental techniques. This is due partly to the relatively simple relationships, partly to the contrast and spectrum sensitivity of the eye and finally to the simplicity of the measuring techniques.

The third trend of the period before the Second World War was the microtechnique introduced by Austrian analysts. This trend which actually initiated the analysis of micro amounts and micro components was not accepted in its time overall seriously, but later it was of high importance and above all changed the view regarding the demands of future analysis.

This represented the stock of knowledge which we had to become acquainted with in the course of our university studies, too. Analytical chemists in practice looked beside gravimetry and titrimetry at best upon photometric methods as applicable techniques and regarded suspectfully every other method. That was the situation when European analysts were reached by the war. The post-war time brought with it numerous challenges for the analysts. The demands fundamentally changed in those times and a period began when the most varied domains of life added to the earlier demands of science and industry, which were also redrafted. The fundamental change in the requests of industry was that, instead of the analysis of the main components of the products, examinations were required in order to detect what kind of contaminants were present in the material. It also became more and more interesting to know in what way the various trace elements and contaminants are distributed in the basic matrix. The examination of the alloys required rather difficult tasks involving on the one hand the analytical verification of the theory of the alloys, which in the thirties developed rapidly, and on the other hand, the prediction of its practical application on the basis of the analytical results.

New challenges

After the Second World War many new industrial branches came into existence and industrial production was significantly accelerated all over the world. This increased production required more work from the analyst, but the quality of the wares produced also increased, causing new qualitative demands on analytical chemistry, and as a consequence the requirements of the analytical measuring techniques changed, too. New situations were created by such industrial branches as *e.g.* the production of semiconductors and of electronic and microelectronic elements of various complexity. The rapid development of pharmaceutical industry raised a new spectrum of requirements, *viz.* that of the examination of the fine structure of organic compounds. Many other cases could be mentioned also, all representing the extended and altered requirements on analytical chemistry. The fundamental change in the demands on analysis can be formulated in most cases as follows: we are not curious whether the analysis of the basic (raw) material produced by us can be solved but we must become acquainted with every single trace and contaminant compounds being present in the system beside the main component, and this is not a question of hobby. Pharmacopoeiae introduced rather early the examination of mini and micro contaminants which may be pernicious even in small concentrations, either by catalysing something in the organism, or by accumulation and enrichment, respectively in the organism, thus becoming the source of illness. But the analytical determination of the mini and micro contaminants in many domains of industry may also serve as protection of the factory itself, because on the basis of these determinations one can conclude with great certainty the synthesis path of the product and in this way the protection of the patent rights of the synthetic process can be ensured.

The analytical demands of industry became manifold and the main trends of them justified the adoption of the Austrian microanalytical trend. But for the performance of the new tasks it was not enough to improve the earlier tools, they had to be replaced by newer ones. New measuring techniques turned up in analytical practice and the number of spectrochemical and electro-analytical methods significantly increased. The field of spectrochemical analysis *e.g.* ranges from the measurement of small interactions requiring radio frequency methods, up to the measurement of very big interaction energies using gamma spectra; this necessitates such technical virtuosity from the researcher that systems must be stabilized in a proportion of $1:10^{10}$. Methods were developed with the help of which surface layers can be etched from the material and so by step penetration into the substance one can examine the special distribution of the components. Staying in the present, let us consider one of the revolutionary steps of industry to be expected in the near future, that of materials coming into existence in the course

of the technical application of ion-implantation which could be examined with the help of a similar process, the ion probe analyzer.

The emission and absorption methods of spectrochemical measuring techniques also have significantly enlarged. The depth of the information obtained has greatly exceeded the hopes of earlier optimistic analytical expectations, too. Let us think on the fact that previously the analysis of an organic substance extended only to the determination of C, H, N, and O in addition to the measurement of a few radical groups and the rather cumbersome determination of the molecular weight. What a great difference is in this field, too. Nowadays by means of mass spectrometers we can determine generally with great accuracy, the molecular weight and with the help of chemiionization and field desorption methods we can do this even when the nature of the molecule (alcohols, aldehydes) or its size would cause difficulty in the simple electronic collision method. With the help of its proton- and ^{13}C -n.m.r. spectra we can state the environment of these atoms using for analytical purposes the formerly only supposed small interactions. We have also the possibility of drawing conclusions regarding the energy state of an atom on the basis of the determination of the kinetic energies of the electrons emitted with a certain energy from the atom mentioned. The XPS and the Auger electron spectroscopy can answer more and more questions. Surface or even deeper layers of solids can be analyzed with electron and ion microprobe techniques and provide industry as well as researchers with information which was earlier quite unthinkable.

Summarizing this, industry made manifold demands on analysis. Analytical chemistry answered this challenge by developing in addition to the earlier classical methods, techniques dealing with the examination of the energies of the various material interactions. In this answer a significant role was played, beside the previously mentioned methods, by electrochemical measuring techniques. Here I think first of all of the great development of the selective ion sensors in the last two decades and the newer and newer methods of voltammetric analyses. I do not wish here to discuss in detail these techniques, either those which are based *e.g.* on the measurement of enthalpy and other new measuring techniques operating on the basis of other physical principles.

The development of the demands of society, which industry tried to satisfy, brought new problems into existence. Mankind became aware that not only the sources of energy and raw materials are limited, as was shown by the Club of Rome, but human activity may contaminate its own surroundings to such an extent that life may be damaged or may become impossible if not enough care is taken. Accordingly, beside the analytical demands of industrial production new requirements arose for examinations of the side effects of this production. So, to the early precautionary measures of water protection in certain countries, as *e.g.* the former Austrian Hungarian Monarchy, new demands for analyses were added with respect to the air and soil.

But independently of all these, in addition to the already mentioned pharmaceutical analyses, the examination of foods has required also more effective and more differentiated methods of analysis. With the development of medical science it was necessary to develop also methods suitable for examining the functioning components in the organism (inorganic components, enzymes, and other organic components). But the great development of clinical analysis was not characterized by a demand for the determination of such a wide variety of components as was shown by industry. Rather, clinical analysis required and requires the analysis of a very great number of samples. Accordingly, the demand of clinical analysis does not involve a wide spectrum of techniques but the exact and reliable measurement of not too many components in a high number of samples.

Agricultural production requires also examinations in large numbers, involving however only a few components, viz. intensive agriculture needs to have beside the continuous analysis of the soil and products, a dynamic soil map to control the mode of production. Far wider is the spectrum of requirements in food analysis where continuous and increasing qualitative and quantitative demands can be observed.

The demands of clinical, agricultural, and environmental analyses shifted the development of chemical analysis from the demands of industry into such directions where the huge number of samples to be analyzed requires a method which needs lesser human involvement. Mechanized, and thereafter computer-controlled automatic analysis systems serve to fulfil this demand. Parallel with the development of laboratory automatic analysis systems the development of automatically operating monitors was also accomplished.

According to the rules of dialectics, such a great development establishes beyond certain quantitative limits, qualitative changes. So it is evident that also in analytical chemistry one has to raise the questions of information theory and in addition to this the problems of the theory of knowledge of analytical chemistry. Professor *Malissa* performed a pioneer work in this respect.

In computer-controlled analysis systems there is a direct possibility for the preliminary working up, processing and interpretation of the obtained analytical signals in contrast to earlier times, when this task involved difficulties. The modern mathematical methods needed to be applied to these purposes and so there was established a new branch called chemometry. Now modern automatic analysis equipment not only works up for us signals as valuable information but if necessary, the whole measuring system can be governed by means of the computer under optimal conditions.

Distribution of social demands

Until now we have not dealt with the question of the effect demands of a society,

in respect of the number of measuring results in the different fields. Here one could collect data from literature.

Permit me to give now a little information about the current demands in Hungary, for through this we can possibly estimate the demands of the other countries, too.

In our country in 1980—1981 there were about 40 million individual clinical analysis data produced. We have data that about 10 years ago in the USA the number of clinical analyses performed amounted yearly to about 8—10 per person. In our case this advances at present at the rate of about 4 data per person. I do not have available newer data from the USA but it is to be expected that the number of the data has increased somewhat in comparison to the data of ten years ago.

Hungarian agriculture underwent a huge development and became significantly intensive. According to the data of 1980—1981 the number of the data obtained in soil examinations was about 10 million/year. These data serve to help the production in agriculture. Calculated for our population, this means ca. 1 datum per person.

The analytical data obtained in industry is nearly impossible even to estimate. We think in yearly average the industry in our country requires about one analytical result per person.

Summing up, we may count in our country about 60 or a little more million analytical results every year.

Prospective trends of development

On the basis of the former description we may survey the present situation. In what direction may the further development be expected? Prophesying in science always involved great dangers of contradiction. Of course, the shorter is the time affected by the prediction the less is the danger. I think we are not very far from the correct prediction if we suppose that in the laboratory equipments of analytical chemistry the age of microprocessors and minicomputers continues and so the measuring technical control as well as the mathematical working up of the obtained signals will occur within the equipments.

In industrial measuring techniques the age of monitors and analytical robots will come, at which reliable measuring results with a long-term stability will be ensured.

This trend of development raises the question, to what trends of research we have to give preference, in order to ensure the acceleration of the development. In my opinion the development of sensors is of decisive importance, now and also in the future, since if their signal formation is wrong, then the data processing can start only with a wrong input and if we feed rubbish into the input of the computer then also through its output rubbish will part.

The other important field of development lies in computer technical software, which investigates the possibilities of signal selection and the improving of the signal—noise relation. Furthermore, it is important also to further develop the various methods of feature selection and pattern recognition.

In addition, in the development of the hardware a great importance must be attributed to the introduction and development of such techniques which perform within the equipments a reliable self-control.

In more and more domains arises the necessity to forward the measuring results in the way of telecommunication. This means an increasing demand from the space probes on to measurements performed inside human beings or animals. These are tasks which nowadays may already be solved and it is to be expected that in the near future they will find a wider application.

I do not dare to prophesy for the further future. However, I would like to point out that due to the mentioned significant developments the demands against the knowledge of analysis greatly changed. To acquire this knowledge during the university studies is not possible anymore, analysts must be trained in the frame of postgraduate teaching.

Unfortunately with the huge demands, the appreciation of analytical chemists has not increased in a parallel way. It would take long to analyze the cause of this, but it is sure that this circumstance must also be attributed to the fact that nonanalytical chemists often think that they are expert in analytical chemistry, since in the course of their training they had learned that simple macro technique which had been called in those days analytical chemistry. But no less dangerous is the approach we meet in increasing number in literature, when mathematicians without any chemical knowledge regard the unknown signal assembly as stochastic signals and work them up without knowing their sense. Also this may contribute in the future to the devaluation of analysts.

Just therefore it is necessary that a new tendency should be supported which is represented by several European professors, first of all by Professor *Malissa*. According to their idea, analysts should take in hand the complex development of analysis and should see that the new analysts should be trained in that way that they become acquainted with every important knowledge of this marginal science.