Short Report

FUNDAMENTALS OF CHEMOMETRICS IN QUANTITATIVE ANALYSIS

Tanganov B.B.
East Siberia State University of Technology
Ulan-Ude, Russia

The article describes a new computer program that enables students to make mathematical processing of research results or laboratory works in interactive mode, and empowers the supervisor to implement monitoring of laboratory work in all the research and educational groups.

Processing of results, evaluation and control of capability of data and permissible errors reproducing, comparison of series of quantitative determinations by chemical and instrumental methods of analysis, mathematical interpretation of linear and nonlinear relationships in the experiments, multilevel modeling of physical and physical chemistry parameters, and etc. are impossible without computer technology. This part of analytical chemistry is called Chemometrics.

At present, the higher education system focuses on students independent work and distance learning, and also to monitoring the implementation of this type of work. We believe the elaborated calculation and monitoring program can help in solving the above said problem not only for part-time or distant learning students, but mainly for full-time two-level training (bachelor's and master's degrees) students according to the Bologna agreements in the field of education.

We have developed a program to control two-stage implementation of student laboratory works on chemical (volumetric and gravimetric) methods of analysis and evaluation of a teacher using a particular algorithm, the results of each student's experiment. It is a series of subprograms, each of which corresponds to one particular laboratory work (16 works in total).

At the beginning of the program the student opens the file of the group, finds his/her name in the list of educational group and selects the number of laboratory work in the general registry, starting an interactive mode. The program asks the student his/her experimental and calculated data in laboratory work, produces separate calculations, compares the data obtained and previously introduces ones to the computer program by the supervisor. In addition, if the difference between the data calculated by the computer and introduced by a student exceeds the allowable difference, the program signals a student an error in calculation or in experiment (e.g., in calculating the characteristics of the mixed solutions), and stops its work in this unit.

If the differences are insignificant, then depending on the relative error of calculation or experiment (the magnitude of which is varied by a supervisor, for example, from 5.0 to 0%), the program asks for data on the fulfilled laboratory works.

On the next stage the subprogram, connected with the quantitative determination of substances in the test sample or a model, gets involved. It compares the data stated by a student with the previously introduced ones by a supervisor. For the data not exceeding the allowable limit, the program signals "the work credited" and it shows an adequate mark on the monitor (from 3.00 to 5.00) for the laboratory work done.

Thus, the student can independently find out how well he made laboratory work.

While working with the program a separate file for a teacher (the supervisor of the practical work) is simultaneously created. It records the name of the student, the time of computer operation, the title of the laboratory work, the data introduced and obtained by a student, the magnitude of relative error and the mark. The teacher controls all the stages of the student's calculations and results with the developed program and monitors the students' laboratory works in all the educational groups.

This method and computer program are tested during several years in carrying out laboratory works and experiments by students of various technological and environmental disciplines and is appreciated in higher education training.