LEARNING TOXICOLOGY THROUGH OPEN EDUCATIONAL RESOURCES

ENVIRONMENTAL DATA PROCESSING AND RESULTS REPORTING

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1. INTRODUCTION

Following the operations flow of the environmental monitoring (Figure 1.), the execution stage, containing information about sampling and analytical measurements were presented in Unit 2, while the evaluation stages, with data processing will be now presented. Thus, Unit 3. contains general information about how we process the environmental data and how we report the monitoring results.

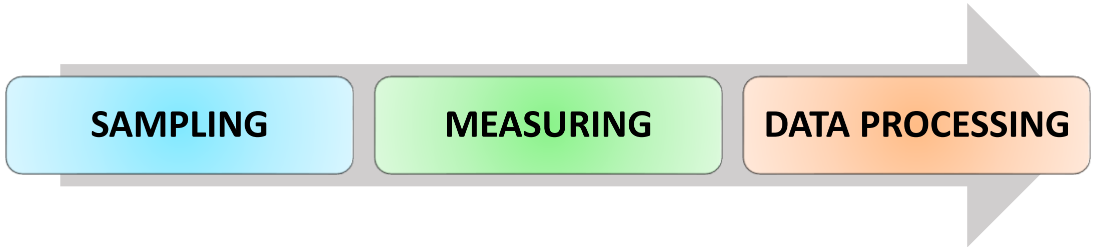

Figure 1. Environmental monitoring flow, execution and evaluation stages.

After passing the unit, you will be able to present the personnel responsible for data processing and results announcing, the stages of the analytical data processing, as well as the monitoring results reporting.

In this respect, Figure 2. indicates the categories of personnel responsible for data processing and results reporting:

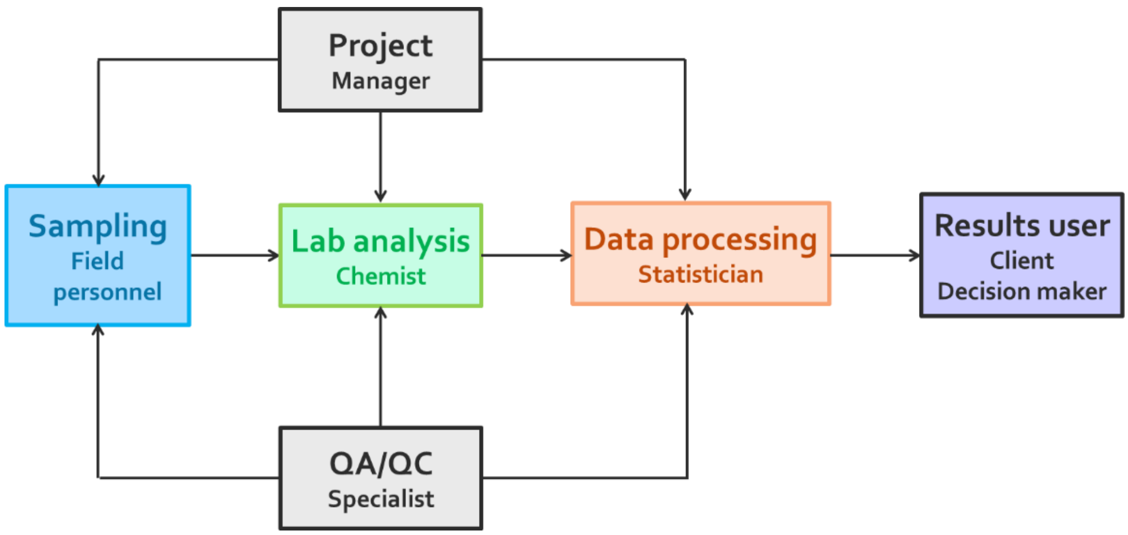

Figure 2. Personnel responsible for data processing and results reporting.

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– persons taking samples on the sites – for the sampling stage;
– chemists and laboratory assistants – for the laboratory analysis;
– *chemists and statisticians – for data processing stage; they further transmit the information to the users of the results, namely the clients and the decision makers.*

2. ENVIRONMENTAL DATA PROCESSING

All the information acquired over the entire environmental monitoring flow are important, of interest for this unit being mostly those marked in italics:

– samples up-taking and sample pre-treatment provides preliminary relevant information;
– measuring the analytical property provides measured values, which we called "data";
– *data are registered in a data acquisition system and are further subject of statistics, in order to ensure trustful and reliable results; that is to validate the dataset;*
– *data processing, based on laws governing different phenomena, the measured signal is transformed into used information, thus, providing monitoring results;*
– *reporting the monitoring results, presenting the obtained results in tables, graphics, diagrams, as functions of other measures, ready to be used by customers.*

Chemometry was introduced in 1972, by Svante Wold, as being a branch of chemistry, which uses mathematics, statistics and other methods based on formal logic, in order to select and project the optimum experimental procedures and to offer the information of chemical data analysis, with maximum relevance. Since 1900's mathematics and statistic methods were used to process measurements data, thus new interdisciplinary sciences were developed in 1970's, like: biometry, medical statistic, psychometry. econometry, technometry, or chemometry,. Moreover, the "Environmetrics" journal was launched in 1990, as the official journal of The International Environmetrics Society (TIES), an Association of the International Statistical Institute.

In most of environmental analysis the true value is hardly unknown, therefore, the true value is estimated by the mean (average) value of repeated measurements. It is estimated that the average value is the best analytical value and. As many repeated measurements we have, as close the mean value is to the true value.

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Statistics make use of a large number of values, but in environmental analysis it is not always possible to obtain such a large number of data, from the same sample. Most of the time maximum 10 repeated measurements can be obtained, therefore, the limited amount of data represents a “selection”, and the result is considered to be an “estimation”.

In order to obtain the reliable results in environmental analysis, errors type, source and extend should be evaluated.

Each stage of the analytical process (sampling, sample preparation, measuring, data processing) is a source of errors, contributing to the final error. These contributions are presented in Figure 3.

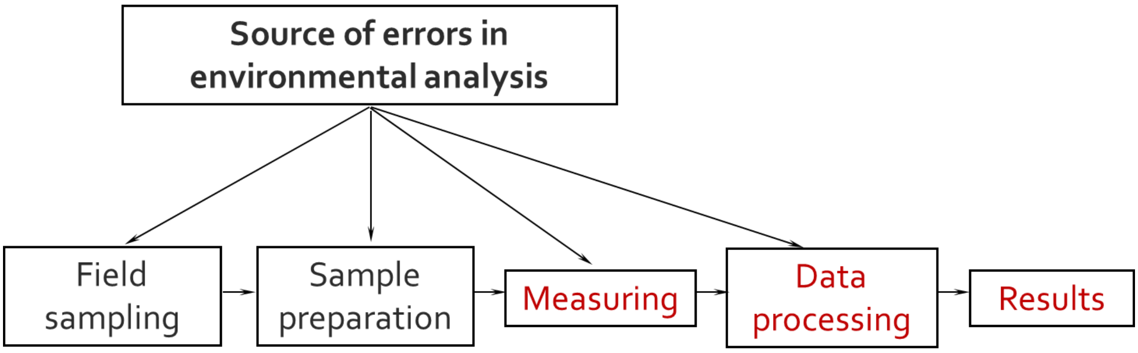

Figure 3. Sources of errors in environmental analysis.

Errors can be classified as follows:

a. according to the expression mode

– *absolute error:* represents the deviation of the individual measured value (X_i) from the mean true value (A), according to Equation (1); if A is unknown, the average of measurements is considered ($\overline{X}$), according to Equation (2).

$$e_a = |A - X_i| \quad (1)$$

$$e_a = |\overline{X} - X_i| \quad (2)$$

– *relative error:* represents the ratio between the absolute value to the true value, considered as standard; is expressed as percentage, according to Equations (3 and 4).

$$e_r = \pm \frac{e_a}{A} \cdot 100\% \quad (3)$$

$$e_r = \pm \frac{e_a}{\overline{X}} \cdot 100\% \quad (4)$$

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b. according to the source and influence on analytical results

– *systematic error (determined)* – sources can be defined (even not always known), like wrong handling of the equipment, wrong readings the signals, working at improper temperature;

– *random errors (un-determined)* – introduced by accident, from individual results falling, their causes are unknown, cannot be determined and eliminated;

– *gross error* – caused by a mal-functionality of the experiment (reagents, equipment, method) and requires the experiment to be restarted.

These errors are reflected in the number of significant reported digits and are observed in the different values obtained from successive measurements. It is important to identify the errors sources and reduce their extend, thus, reporting trustful and reliable results.

3. MONITORING RESULTS REPORTING

Environmental control generates lots of data on samples from different analytical methods. Such data can show trends, correlations, need for reduction. Univariate or bivariate methods of data processing fail to show coherence between the data.

Data are processed, are subject to calculations, based on physical-chemical laws. The aim is to expressed the monitoring results as concentration of the analytes / pollutants (or any other monitoring parameter), in units according to the regulations.

Further, the monitoring results are announced in different ways:

- as such, in *table format*;
- as *bi-dimensional graphs*, for a single monitored parameter, either as evolution of the pollutant concentration over time, C_A=f(t), or as evolution in space, C_A=f(s);
- as *multi-dimensional graphs*, for more parameters that can be correlated.

For example, Figure 4. shows a multi-dimensional graph, correlating sulphur and nitrogen oxides with the pH, for a given location.

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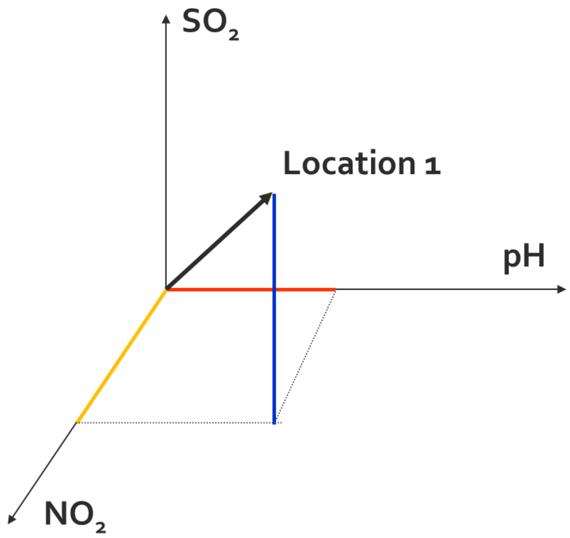

Figure 4. Dependence of sulphur and nitrogen oxides with pH.

Everywhere more and more data are produced and presented, making it more difficult to realise what is going on, and to get an overview of the problem. To make intelligent decisions multivariate approaches are indispensable.

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