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Multicriteria decision analysis in ranking of analytical procedures for aldrin determination in water

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ABSTRACT

The study presents the possibility of multi-criteria decision analysis (MCDA) application when choosing analytical procedures with low environmental impact. A type of MCDA, Preference Ranking Organization Method for Enrichment Evaluations (PROMETHEE), was chosen as versatile tool that meets all the analytical chemists – decision makers requirements. Twenty five analytical procedures for aldrin determination in water samples (as an example) were selected as input alternatives to MCDA analysis. Nine different criteria describing the alternatives were chosen from different groups – metrological, economical and the most importantly – environmental impact. The weights for each criterion were obtained from questionnaires that were sent to experts, giving three different scenarios for MCDA results.

The results of analysis show that PROMETHEE is very promising tool to choose the analytical procedure with respect to its greenness. The rankings for all three scenarios placed solid phase microextraction and liquid phase microextraction – based procedures high, while liquid–liquid extraction, solid phase extraction and stir bar sorptive extraction – based procedures were placed low in the ranking. The results show that although some of the experts do not intentionally choose green analytical chemistry procedures, their MCDA choice is in accordance with green chemistry principles. The PROMETHEE ranking results were compared with more widely accepted green analytical chemistry tools – NEMI and Eco-Scale. As PROMETHEE involved more different factors than NEMI, the assessment results were only weakly correlated. Oppositely, the results of Eco-Scale assessment were well-correlated as both methodologies involved similar criteria of assessment.

1. Introduction

Green analytical chemistry is laboratory philosophy that recognizes the certain analytes determination process as an environmental problem. During analytical procedure, certain compounds can be emitted to the environment [1]. Application of green analytical chemistry means the reduction of procedural environmental impact [2]. The most common methods of reducing negative influence is the application of miniaturized extraction techniques at the stage of analytical sample preparation and miniaturization of analytical instruments [3,4]. The other approach is elimination of sample preparation step by application of direct analytical techniques, which in fact can be applied rather seldom [5,6]. These solutions in greening the analytical procedures are relatively well established and have been reviewed exhaustively [7–10].

One of the main problems in the field of green analytical chemistry is the assessment of analytical procedures greenness. There are several still very vital questions. How to measure the procedural greenness? How to compare the environmental impact of methodologies to choose the most environmentally friendly one? Can an universal procedure be developed to help or guide in procedure selection for the given purpose? There are few assessment methods available, each of them has its own advantages and disadvantages. The only assessment procedure, that is brought into a broader laboratory practice, is labeling with NEMI symbols [11]. NEMI symbol is easy to read circle with its fields filled green (or not) if certain assumptions are fulfilled. These are generation of wastes in the amount lesser than 50 g, no corrosive environment is present and there are no hazardous or dangerous chemicals used during analytical procedure. The main drawback in NEMI application is the need to search the hazardous substances lists to check if any of chemicals used in the procedure is present on these lists, which is time-consuming task. The other NEMI drawback is that the information carried by the NEMI symbol is not quantitative. This problem is partially solved when NEMI modification

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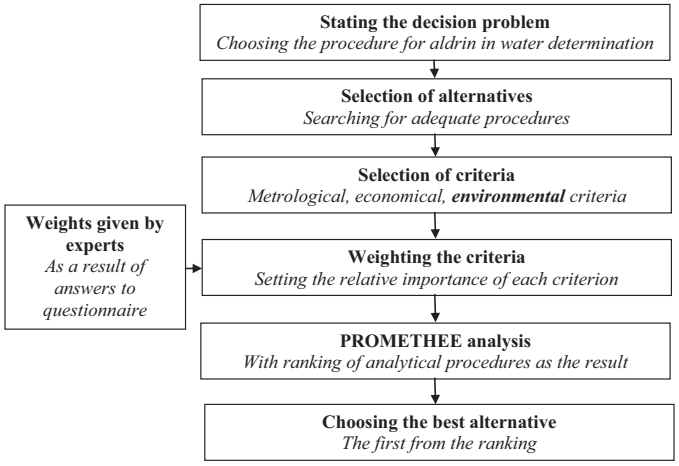

Fig. 1. The scheme of analytical methodologies assessment procedure with multicriteria decision PROMETHEE technique.

proposed by de la Guardia and Armenta is applied [12]. In such a case NEMI symbol carries the semi-quantitative information about threat in each of its categories. The other approach in assessment of analytical procedures greenness is application of Eco-Scale [13]. The Eco-Scale involves many factors that can have negative impact on the environment such as the amount and the type of any chemical used in the procedure, the mass of generated waste, the occupational exposure and energy consumption. The result of Eco-Scale application is the number lower than one hundred, the closer the values to one hundred the more green analysis. The main disadvantage of application of Eco-Scale is the fact that the result is the number which in fact involves many parameters but it does not carry any information about the nature of threats related to the analytical procedure. The latest approach, that gives the possibility to classify the analytical procedures taking into consideration their environmental impact, is the application of multivariate statistical techniques [14]. The techniques such as self-organizing maps allow to group the analytical procedures according to their similarity when environmental, metrological and technical parameters, describing the analytical procedure, are considered. The drawback of multivariate statistics application is tedious assessment procedure and that it might be applied to compare limited amount of procedures [15]. It is clear that green analytical chemistry still needs the reliable procedural assessment methods.

Multicriteria decision analysis is used in environmental science and environmental management [16]. It has been successfully applied to select proper remediation procedure for contaminated mine treatment [17], method of water disinfection [18] or choosing priority areas for environmental monitoring [19]. All these examples involve social, environmental, economical, technological criteria during the decision process. The Preference Ranking Organization Method for Enrichment Evaluations (PROMETHEE) methods are chosen from available multicriteria decision analysis methods because of two reasons. First of all they are easy to apply compared to other methods (such as Elimination and Choice Expressing Reality – ELECTRE or Analytic Hierarchy Process – AHP) because PROMETHEE methods require fewer parameters from decision makers. They also rank alternatives as well as identify the best alternative, whereas the previously mentioned utility theory methods only identify the best alternatives [17]. Ranking alternatives seems to be the most important because there are 25 alternatives taken into consideration and it is not only important to know which is the best among all but also to make it possible to compare all the alternatives. It is important aspect when concerning PROMETHEE as the tool in assessment of green analytical chemistry metrics. It seems to be important to mention that there were several rankings of MCDA methods published [20] and PROMETHEE is concerned to be one of the top in alternatives ranking, easiness of use and potential of future development.

The aim of the study is to investigate the possibility of application of multicriteria decision analysis (PROMETHEE) as the analytical procedure assessment tool in the light green analytical chemistry. The second aim is to show that environmental impact aspects should be considered when making decision of choosing the analytical procedure for the given purpose. Some remarks on choosing the best procedure will be also provided.

2. Materials and methods

The general scheme of the presented multicriteria decision analysis assessment approach is shown in Fig. 1. Briefly, after stating the decision problem, the set of alternatives (the possible options) is identified. Then the important aspects – criteria, have to be defined, together with their relative importance by assigning weights to the criteria.

2.1. The PROMETHEE method

The PROMETHEE (Preference Ranking Organization Method for Enrichment Evaluations) is one of the leading MCDA (Multi-Criteria Decision Aid or Analysis) methods that was developed by Brans and Vincke in 1985 [21]. The methodology is successfully used in various areas such as business, public administration, industrial location, medicine or tourism [22].

PROMETHEE is a family of outranking methods that consist of PROMETHEE I which generates partial ranking, PROMETHEE II for complete ranking of alternatives, PROMETHEE III for ranking based on interval, PROMETHEE IV for ranking (partial or complete) of alternatives set of viable solutions is continuous, PROMETHEE V for problem with segmentation constraints, PROMETHEE VI for human brain representation. There are also additional methods: PROMETHEE GDSS for group-decision making, PROMETHEE TRI used when sorting problems appear and PROMETHEE CLUSTER for nominal classification [22]. In the presented paper PROMETHEE II is going to be applied, because the ranking of many alternatives is the most desired analysis output from our point of view.

The principle of PROMETHEE II is based on pairwise comparison of alternatives along each criterion. To implement the methodology it is required to have two types of information: weights of the criteria and the preference function. In order to obtain information within the criteria, a preference function for each criterion, expressing the difference in performance of alternative a over alternative b must be identified, adopting as a result the pairwise comparison approach [20]. It is also requested to have clear and understandable (by both decision-maker and analysts) information between the criteria and information within each criterion.

When A of n alternatives $(a_1, a_2, \ldots, a_n)$ have to be ranked and G of k criteria $(g_1, g_2, \ldots, g_k)$ have to be maximized (or minimized) the resulting problem has the form as shown [17]:

$$\max\{g_1(a), g_2(a), \ldots, g_k(a) | a \in A\}$$

Some criteria might be maximized whereas others might be minimized, the goal of the decision-maker is to identify an alternative which is optimizing all criteria.

The detailed mathematical description of PROMETHEE was presented by its developers Brans and Vincke in [21].