A Simulation of the Impact of Waste Batteries on Ecosystem Reliability

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Abstract. In order to assess the impact of a battery's multi-element composition on the state of the environment, a new approach is proposed through the determination of the reliability of ecosystems, one which makes it possible to obtain quantitative indexes of the stability and losses of natural ecosystems. These data can be used as indicators of the state of the environment, and hence as the assessment of an environmental component important for determining the actual impact of the multi-element composition of batteries. On the basis of such indicators, which can be obtained using the SimaPro software, it is possible to calculate thresholds beyond which negative phenomena occur, as well as to predict and simulate situations, to carry out the mapping of sources of risks, and to monitor changes. This will allow the causes of these changes to be identified or to determine the factors that slow down or retard the approach of ecosystems to a critical state, i.e. to develop preventive measures to avoid disasters. The eco-indicator 99 is one such method that allows us to accept a single estimate for a whole product – the so-called ecological index. It is the sum of all individual eco-points or partial indexes for all life-cycle processes. The computational procedure is carried out by summing up the results of weighing the phases of the life cycle.

1. INTRODUCTION

When used batteries enter the stream of solid household waste and, due to mechanical damage and corrosion upon disposal, their hermetically sealed casing is broken and this results in the release of toxic substances (Bernstad *et al.*, 2011). The high concentrations

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of lead, cadmium and other heavy metals and compounds in batteries that have dangerous properties subsequently leads to environmental pollution and the loss of the ecological reliability of the ecosystem (Ishchenko *et al.*, 2019). The reliability of the ecosystem is defined as the ability of the ecosystem and its individual parts to withstand the fluctuations of external factors and to maintain its structure and functional characteristics.

2. CLASSIFICATION AND STANDARDIZATION OF CHEMICAL CURRENT SOURCES (CCS)

Chemical current sources are divided into primary and secondary batteries (Bigum *et al.*, 2013). Primary CCSs are for single-use and contain a certain amount of active substances which after use means that the batteries lose their ability to operate. Secondary CCSs or rechargeable batteries, are designed for multiple use. When discharged, the rechargeable battery operates as a primary CCS, at the same time, the conversion of the chemical energy of the initial active substances into electrical energy takes place. Rechargeable batteries can be discharged and recharged multiple times (Camara *et al.*, 2012).

To unify the CCSs, international standards have been developed which mark the power sources by physical parameters and chemical composition. For example, the American National Standards Institute (ANSI) classifies CCSs by physical parameters without indicating their chemical composition (Ishchenko *et al.*, 2018). In the old ANSI system, the designation began with a letter (or letters), which means (their) system and standard size, and then they denote the numbers that indicate the size. In the new standards, the designation begins with digits which generally mean standard size (Janz, 2010; Khan and Kurny, 2012). The International Electrotechnical Commission (IEC) classifies chemical current sources by designating forms, standard sizes and electrochemical systems. Standard designations of primary CCSs are determined on the basis of digits (number of series- connected elements, standard size) and letters (electrochemical system).

3. METHODS FOR THE DETERMINATION OF THE COMPOSITION OF MULTI-ELEMENT BATTERIES

The study was conducted on the "EXPERT 3L" model – a device for making precision measurements in stationary and mobile laboratories. The "EXPERT 3L" energy dispersion X-ray fluorescent analyzer (hereinafter referred to as "Analyzer") is intended for the measurement of the mass fraction of elements with atomic numbers from 12 (magnesium) to 92 (uranium) in homogeneous monolithic samples of metal alloys (ingot, details, foil, wire). For the purpose field, the Analyzer is a universal direct-reading device that operates without changing the calibration and reconfiguration for determining the mass particles (%) of chemical elements in samples of unknown composition and arbitrary form.

4. RESULTS AND DISCUSSION

In order to make a quality analysis, it is sufficient by means of the X-ray spectrometer to determine the energy of the XPI-lines from the object and, according to their value, to identify the existing elements. The quantitative analysis is based on the proportionality predicate between the intensity of the XPI-element and its content in the control object. Average values of the chemical composition of the batteries in the study are shown in Table 1.

Table 1. *Elemental composition of the study batteries*

Chemical element	Composition, % by weight		Concentration of chemical substance	
	molten salt battery	alkaline batteries	molten salt battery	alkaline batteries
Positive pole				
K	–	3.357	–	$3{\times}10^{-4}$
Mn	0.206	0.159	$2{\times}10^{-5}$	$2{\times}10^{-5}$
Fe	92.812	61.522	$93{\times}10^{-3}$	$62{\times}10^{-3}$
Ni	–	34.962	–	$35{\times}10^{-3}$
Cl	1.856	–	$2{\times}10^{-4}$	–
Ca	2.294	–	$2{\times}10^{-4}$	–
Cr	0.050	–	$5{\times}10^{-6}$	–
Mn	0.206	–	$2{\times}10^{-5}$	–
Zn	1.370	–	$1{\times}10^{-4}$	–
Sn	1.413	–	$1{\times}10^{-4}$	–
Insulation				
K	–	11.877	$12{\times}10^{-3}$	–
Mn	–	0.319	$3{\times}10^{-5}$	–
Fe	–	0.077	$8{\times}10^{-6}$	–
Zn	–	87.728	$88{\times}10^{-3}$	–
Casing				
Fe	97.467	0.266	$97{\times}10^{-3}$	$3{\times}10^{-5}$
Cu	–	70.421	–	$70{\times}10^{-3}$
Zn	–	29.320	–	$29{\times}10^{-3}$
Ca	1.296	–	$1{\times}10^{-4}$	–
Cr	0.066	–	$7{\times}10^{-6}$	–
Mn	0.357	–	$4{\times}10^{-5}$	–
Sn	0.814	–	$8{\times}10^{-5}$	–
Anode				
Mn	–	0.062	–	$6{\times}10^{-6}$
Cu	–	31.635	–	$32{\times}10^{-3}$
Zn	–	68.393	–	$68{\times}10^{-3}$

Table 1. (cont'd)

Chemical element	Composition, % by weight		Concentration of chemical substance	
	molten salt battery	alkaline batteries	molten salt battery	alkaline batteries
Cathode				
K	–	0.747	–	7×10^{-5}
Ti	–	0.647	–	6×10^{-5}
Mn	45.889	0.222	46×10^{-3}	2×10^{-5}
Fe	0.915	63.455	$9 \times 10^{--5}$	63×10^{-3}
Ni	–	34.859	–	35×10^{-3}
Zn	53.196	0.070	53×10^{-3}	7×10^{-6}
Anodic conductor				
Cl	21.345	7.368	21×10^{-3}	7×10^{-4}
K	10.383	0.675	10×10^{-3}	7×10^{-5}
Ca	5.135	0.200	5×10^{-4}	2×10^{-5}
Ti	3.350	0.884	3×10^{-4}	9×10^{-5}
Mn	7.436	0.084	7×10^{-4}	8×10^{-6}
Fe	26.620	22.79	27×10^{-3}	23×10^{-3}
Ni	–	7.854	–	8×10^{-4}
Zn	23.820	60.092	24×10^{-3}	60×10^{-3}
Rb	0.273	0.002	3×10^{-5}	2×10^{-7}
Zr	0.408	0.009	4×10^{-5}	9×10^{-7}
Sn	0.459	0.420	5×10^{-5}	4×10^{-5}
Pb	0.770	0.943	8×10^{-5}	9×10^{-5}
Negative pole				
K	–	3.357	–	3×10^{-4}
Mn	–	0.159	–	2×10^{-5}
Fe	97.729	61.522	98×10^{-3}	62×10^{-3}
Ni	–	34.962	–	35×10^{-3}
Zn	–	2.041	–	2×10^{-4}
Ca	1.271	–	1×10^{-5}	–
Cr	0.081	–	8×10^{-6}	–
Sn	0.919	–	3×10^{-6}	–
Plastic	1.6000	1.000	–	–
Paper, cardboard	7.6000	6.000	–	–
Other elements	0.600	0.135	–	–

By adjusting the hazard level indexes , taking into account the percentage (wt.%) of each element of the batteries in the study, it is possible to estimate the consolidated figure of the danger level of the elemental composition of the batteries.

It is assumed that the distribution of battery components according to the types of systems used in the analyzed sample reflects their distribution in solid municipal waste. To determine the elemental composition of batteries that have an impact on the environment, a Pareto analysis was made. It can be concluded that the strongest environmental impact is caused by the internal content of the batteries. Based on this fact, we will analyze the effect of the battery life cycle on the state of the environment.

As computational procedures used to aggregate data in the influence of elemental composition of batteries, environmental models are used to compare different contributions to the same environmental problems. This task can be achieved by using the factor equivalence provided by the models (Fig. 1).
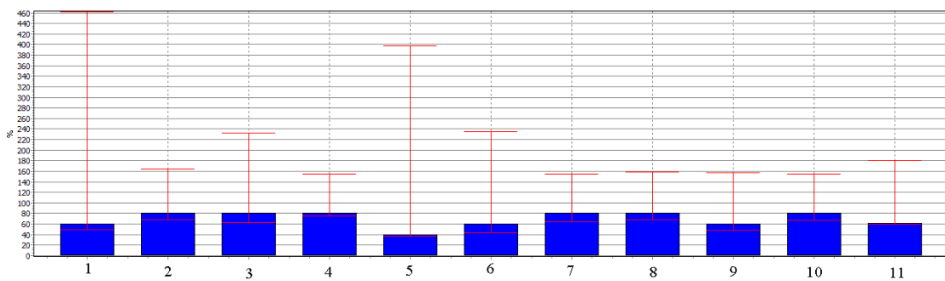

Fig. 1. *Assessment of the elemental battery composition impact on the environment: 1 – cancerogene; 2 – respiratory organics; 3 – respiratory inorganics; 4 – climate change; 5 – radiation; 6 – ozone layer; 7 – eco-toxicants; 8 –eutrophication; 9 – soil contamination; 10 – mineral resources; 11 – mineral deposit*

From this graph (see Fig. 1), the characteristic results of the specific impact of the elemental composition of batteries on the components of the environment is clearly discernible, as are scenarios for the generation and distribution of waste. This suggests that transport is dominant with some categories of impact, while at the end of the life cycle, it is other factors that predominate; all impacts are reflected on a 100% scale. As can be seen from the graph above, the strongest negative impact on the environment will arise from waste, that is, the penetration of pollutants into the soil, and therefore having a corresponding impact on both the eco-toxicity level and climate change. This is due to the fact that the penetration of pollutants through the soil layer to plants, and then to the atmosphere, is accompanied by phenomena such as the accumulation of harmful substances which enter underground and surface waters, and also cause considerable air pollution, making a corresponding negative contribution to climate change.

5. DETERMINING THE RELIABILITY OF ECOSYSTEMS

In light of ensuring the transition of society to the principles of sustainable development, it is important to assess the risk of losses, the destruction of ecosystems, which is closely connected with their stability (Grime, 1979; Hopper, 2009). Ecosystem stability

is seen as the ability to maintain its structure and the nature of its functioning in space and time despite changes in the environment (Moreno-Merino et al., 2015). The theoretical foundations of stability are substantiated in the classical works of Poincare, Lyapunov, Lagrange, Svirizhev and Logothete which are based on the estimates of the assimilation and transformation of energy and information, that is, the laws of thermodynamics of the functioning of ecosystems, synergetics, and entropy indicators applied to open systems (Polygalov *et al.*, 2015).

These authors have shown that natural ecosystems, although directed to an equilibrium state in their development, cannot exist in this state and require additional energy which is provided at the expense of dissipative processes (Gorshkov, 1995; Glensdorf and Prigozhin, 1973). In mathematical terms, changes in the behavior of ecosystems are described by nonlinear equations. These processes occur as fluctuation changes that cause turbulence and can lead to disaster, that is, the destruction of the ecosystem (Hsing Po Kang, 2012).

In our study, the basic method for determining the reliability of ecosystems was the creation of models to estimate the synergistic action of the elemental composition of batteries on ecosystems. The main parameters for the model, which were obtained during experimental investigations and processed using the SimaPro software, are required to determine ecosystem stability. The coefficient of synergy P is determined by the following dependence:

$$P = \frac{S_{Cd+opr}}{S_{Cd} + S_{opr}} S_0 \tag{1}$$

where:

S_0 – the ratio of the factors of influence on the ecosystem for the control variant (each of them is defined as the ratio of pollutants absorption rate to the rate of its outflow);

S_{Cd+opr} – the same ratio with combined impact of the elemental composition of the batteries;

S_{Cd} and S_{opr} – the ratio of factors for the independent influences of each of them.

Substituting the data obtained with SimaPro, we obtain the value of $P = 0.752$. If $P = 1$, it is clear that there is no synergy in the action of various factors on the parameters. If $P < 1$, then this may indicate a significant contribution of synergy, that is, the enhancement of the factors compared to the action of each of them separately. If $P > 1$, then we are dealing with antagonism, that is, with the phenomenon when the first factor reduces the negative effect of the next, or vice versa. Thus, a scheme is developed and a parameter is introduced to estimate the degree of interaction of various factors through the above-mentioned coefficient – P.

When the period of observation is long, one can calculate and estimate the stability factor. It is also worth noting that the ratio of absorption and outflow rates of the pollutants and the element of mineral nutrition is proportional to the biomass of the biota and the accumulation coefficient in the ecosystem. Thus, we have an ecosystem that is under the influence of pollutants – $Y(x)$ and $Z(x)$, which varies with time x; a_{12} is the rate of absorption of pollutants (in proportion to the absorption rate of nutrients, (e.g. potassium); a_{21} is the rate of outflow of pollutants, for example,

through entropy. The solution of two differential equations for this model is:

$$Y(x) = \frac{Y_0}{a_{12} + a_{21}(a_{21} = a_{21}\exp[-(a_{12} + a_{21})x])} \tag{2}$$

$$Z(x) = \frac{Y_0 a_{21}}{a_{12} + a_{21}(\exp[-(a_{12} + a_{21})x])} \tag{3}$$

Based on the above, when the observation time is long, the reliability factor can be estimated as follows:

$$F_b \approx \frac{a_{12}}{a_{21} + a_{12}}; \quad F_w \approx \frac{a_{21}}{a_{12} + a_{21}}$$

$$F_b \cong \frac{a_{12}}{a_{12} + a_{21}}; \quad F_w \cong \frac{a_{21}}{a_{12} + a_{21}}; \quad \frac{F_b}{F_w} = \frac{a_{21}}{a_{12}} \tag{4}$$

where F_b is the reliability factor for the soil; F_w is the reliability factor for water. The ratio of absorption and outflow rates of pollutants and elements of mineral nutrition is proportional to the biomass of the biota and the accumulation coefficient in the "soil-biota" system. This means: the larger the biomass of the biota and the coefficient of accumulation of pollutants by the biota, the higher the ratio of absorption and outflow rates of pollutants, and hence the flow of nutrients from water to the biota biomass. Here, one can clearly see the relationship of the parameter of reliability with the content of pollutants and the rates of absorption and outflow of the pollutants.

Let us construct a model of the synergistic action of battery multi-element composition on the soil. As shown above, the parameters of the reliability factors are determined by the following formula:

$$F_b \cong \frac{a_{12}}{a_{12} + a_{21}}; \quad F_w \cong \frac{a_{21}}{a_{12} + a_{21}}; \quad \frac{F_b}{F_w} = \frac{a_{21}}{a_{12}} \tag{5}$$

The impact of any pollutant on these parameters, and therefore on the state and ecological safety of biota, can be specified in this way. Obviously, the flow of pollutants to biota should change their exchange rate. Then, on exposure to pollutants, the expressions for rates can be written as follows:

$$a_{12} = a_{12}c, \quad a_{21} = a_{21}d \tag{6}$$

where c and d are coefficients of pollutant influence on the parameters of the reliability according to the amount of pollutant.

The parameter S – area of contamination under the influence of the pollutant SR which will take the form:

$$S_R = \frac{12}{S_c}d \quad \text{or} \quad \frac{S_R}{S} = \frac{c}{c} \tag{7}$$

The ratio of S_R/S values can serve as the degree of the pollutant's influence on the stability parameters. The more this ratio differs from unity, the greater the degree of the pollutant's impact on the biota.

In the event of the simultaneous action of several factors, one can obtain an expression for determining the pollution area S_{total}:

$$S_{total} = S\left(\frac{\sum_i^n \text{cm}}{\text{dn}}\right) = \frac{S_1 \times S_2 \times \ldots \times S_i}{S} \quad \text{or} \quad \frac{S_{1+2=\ldots=n}S^2}{P_2 S_1 \times S_2 \times \ldots \times S_i} \qquad (8)$$

In general, under the influence of n-pollutants, the formula for determining the area of pollution, through the evaluation of synergy and a consideration for the parameters of stability, will be as follows:

$$S_n = \frac{S \sum S^{n-1}}{\prod S_i} \qquad (9)$$

Applying the Formulas (5) and (9) for assessing the synergy (interaction) of the elemental composition of a battery, according to the results of the experiment, it can be determined that the value S_n, the area of pollution, is 16.75 ± 0.027 m^2.

To determine the actual environmental impact of battery elemental composition, and based on the hypothesis that the composition of the batteries can be represented as a set of chemical elements (presented in Table 2), we select a portion of the unit area. We draw the upper limit parallel to the surface of the soil at a height H, approximately equal to the triple height of the trees h. At a certain depth R, outside the layers of the root system location, we will draw a lower limit. A parallelepiped formed in such a way will be considered as an object of pollution. Since the exchange of energy and matter does not occur through the side faces, the solar radiation and carbon dioxide come from above the surface, while water vapor, for example, is removed from the lower face. Similarly, the mentioned exchange processes occur through the lower face. At the same time, everything that enters the system refers to its input impacts, and everything that is removed from it – either to losses or to the alienated final product. Denote the upward vertical coordinate by x, placing its origin (point 0) on the surface of the soil. Time is denoted by t. In this case, all model variables will depend on two arguments x and t. At each time point in the system, there is a vertical distribution of characteristics of the vegetation cover, as well as of different substances – water in the soil, ammonium ions and nitrates in the soil profile, soil temperature, contamination by pollutants and sediments, etc. In the above-ground part of the system, there is also a vertical distribution of various parameters – anthropogenic pollution, radiation, temperature and humidity of air, leaf temperatures, the carbon and nitrogen concentrations in phytoelements, etc.

Knowing the chemistry of the soil contamination process and the values for the contamination itself, we calculate the volume of contaminated soil. The volume of the contaminated soil will be deduced from the total volume of pollution caused by one battery per unit area:

$$V_{zac} = S_n \cdot A \qquad (10)$$

where S_n is the area of contamination under the action of n-pollutants, obtained through the synergistic assessment and taking into account the stability parameters (calculated by Formulas (8) and (9); A is the limit of contamination of the unit area

with the elemental composition of the battery, calculated by the formula:

$$A = H + r + K \tag{11}$$

where:

H – the triple tree height: $h \times 3$ (h is taken to be the average tree height – 15 m);

r – the depth of the root system;

K – some value outside the root system (according to the experimental studies, we assume it to be equal to 3), based on the value of the soil pollution index which is calculated by the formula:

$$Z_c = \sum_{1}^{n} K_c - (n - 1) \tag{12}$$

where $K_c = \frac{K_j}{MPC}$ is the concentration coefficient of a chemical substance, K_j is its actual contents in the battery, n is the number of summation elements whose content in the soil exceeds the MPC (MPC – Maximum Permissible Concentration).

$$V_{total} = 16.75 \times 53 = 887.75 \text{ m}^3 \tag{13}$$

For the soil, this value is: $V_{total} = 16.75 \times 8 = 134 \text{ m}^3$. Thus, we have determined the actual value for the volume of pollution of the environment as well as the area of soil contamination, based on the ecosystem reliability theory.

6. CONCLUSIONS

A new approach is proposed to assess the impact of the multi-component composition of batteries on the state of the environment through the determination of ecosystem reliability. This approach provides an opportunity to obtain quantitative indexes of the stability and losses of natural ecosystems, which can be used as indicators of the state of the environment and, consequently, for the evaluation of an environmental component that is important to determine the real impact of the elemental composition of batteries. On the basis of such indicators, which can be obtained using the SimaPro software, it is possible to calculate thresholds beyond which negative phenomena occur, to predict and simulate situations, to map sources of risks, to monitor changes, and ultimately allow the identification of the causes of these changes or determine the factors that slow down or retard the approach of ecosystems to a critical state, that is to develop preventive measures to avoid disasters.

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