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Life Cycle Inventory (LCI) Stochastic Approach Used for Rare Earth Elements (REEs), Considering Uncertainty

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Abstract. The purpose of the paper is to present the results of the stochastic modelling with uncertainty performed with the use of Monte Carlo (MC) simulation with 10,000 cycles and a confidence interval of 95 %, as recommended. Analysed REEs were fitted by lognormal distributions by using the Crystal Ball® (CB) spreadsheet-based software after defining the geometric mean value (μg) and the standard deviation (σg), automatically calculated (matches) the lower, as well as, upper boundaries of lognormal distribution. The number of replications of a simulation affects the quality of the results. The principal output report provided by CB and presented in this study consists of the graphical representation in the form of the frequency chart, percentiles summary, and statistics summary. Additional CB options provide a sensitivity analysis with tornado diagrams. The data that was used for MC simulation of the LCI model includes available and published data concerning associated with the REEs. This paper discusses the results and show that the adopted approach is applicable for any REEs used in the LCI studies under uncertainty. The results obtained from this study can be used as the first step in performing a full LCA analysis and help practitioners as well as decision-makers in the environmental engineering and management.

Keywords: Life cycle inventory (LCI), Stochastic approach, Rare earth elements (REEs)

1. Introduction

The REEs are grouped into two different categories on the basis of their atomic numbers. REEs with atomic numbers 57-63 are classified as light-rare earths (LREEs), and REEs with atomic numbers 64-71 are classified as heavy-rare earths (HREEs) [1]. According to Xie et al. [2] the term "rare" earth is a misnomer; because they are relatively abundant in the Earth's crust, as well as they are typically dispersed and only rarely occur in concentrated and economically exploitable mineral deposits [3].

The Socialist Republic of Vietnam has many of mineral resources located in the northern part of the country [4]. The large resource of rare earth metals in Vietnam is located in the Namxe rare earth deposit which belongs to Namxe commune, Phongtho district, Laichau province (Fig. 1) [5]. Based on the previous studies presented in [6], the rare earth deposit contents include about 80 different minerals.

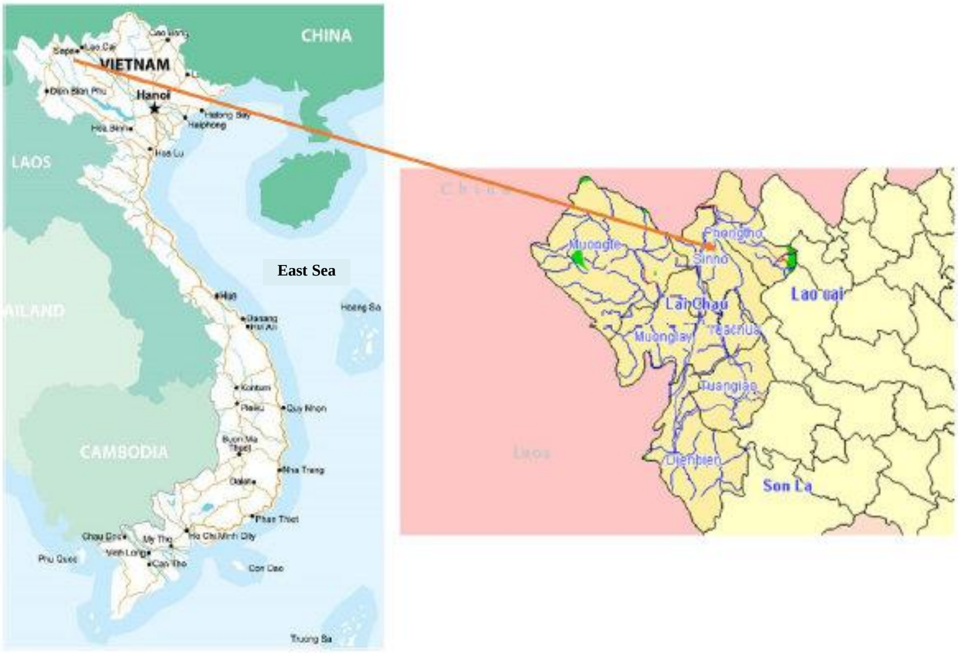

Fig. 1. Location of Namxe rare earth deposit [5, 7, 8].

2. Materials and Methods

2.1 Uncertainty analysis

In this study uncertainty is performed by using the Monte Carlo (MC) simulation The applicability of the MC approach for assessing parameter uncertainty was presented as follows by Warren-Hicks and Moore [9]:

1/ select a distribution to describe possible values of each parameter;

2/ specify properties of each parameter;

3/ generate data from the distribution;

4/ use the generated data as possible values of the parameter in the model to produce output.

Ribal et al. [10] quoted the definition of uncertainty given by Huijbregts [11] which is as follows: "Uncertainty is defined as incomplete or imprecise knowledge, which can arise from uncertainty in the data regarding the system, the choice of models used to calculate emissions and the choice of scenarions with which to define system boundaries, respectively". Suter [12] proposed uncertainty definition as follows: „imperfect knowledge concerning the present of future state of the system under consideration". This definition is similar to the definition given in Reinert et al. [13], and is as follows: „process that assesses the imperfect knowledge concerning the present of future state of the system under study; may be qualitative and/or quantitatively addressed.

In our case the REEs were fitted by lognormal distributions with σg equal 1.1 obtained by using the Crystal Ball® (CB) spreadsheet-based software. The graphic illustration of log-normal probability distributions used to assess the La, Ce and Nd, offered in CB software (Lognormal Distribution tab windows), are shown in Figures 2, 6 and 10, respectively. The simulation outputs after 10,000 runs have been given in the form of frequency forecast charts (Figs. 3, 7 and 11), and statistic reports (Figs. 4, 5, 8, 9, 12 and 13, respectively).

In order to obtain an accurate value, the MC method should be based on a large number of simulations [13]. The number will vary from problem to problem at least in hundreds and, even better, in thousands [14], through 5000 runs [21] to up 10,000 runs [10, 15, 16]. Further guidance to MC simulation is provided by the ILCD handbook - General guide for Life Cycle Assessment - Detailed guidance [17]. Each realization, or trial, involves random selection of a value for each uncertain quantity (according to a probability or frequency distribution).

Probabilistic methods are distinguished from deterministic methods in that exposure is characterized not as a point estimate but as a probability distribution (or frequency distribution) of possible estimates, based on the use of distributions to characterize some or all of the uncertain input quantities [18]. Moreover, probabilistic methods improve accuracy in risk characterization by capturing a more realistic range of possible outcomes than from deterministic methods in that deterministic methods [18].

The data used in the current study is obtained from the Deliverable D1.2 Report and Deliverable D1.3 Report – with both coming from the ENVIREE (ENVIronmentally friendly and efficient methods for extraction of Rare Earth Elements from secondary sources) - funded grant within the second ERA-NET ERA-MIN Joint Call Sustainable Supply of Raw Materials in Europe 2014 [19]. The each REEs analyzed in this study is independent (uncorrelated) of the others and comes from the same source, in this case from laboratory. A stochastic (probabilistic) analysis considering uncertainty and using MC, has been performed on three selected REEs, namely Lanthanum (La), Cerium (Ce) and Neodymium (Nd).

This project aims to increase the knowledge on the stochastic modelling (used random probability distribution) considering uncertainty and performed by the use of the Monte Carlo (MC) simulation.

The graphic illustration of log-normal probability distributions used to assess of the La, Ce and Nd, adopted in CB software (Lognormal Distribution tab windows), are shown in Figures 2, 6 and 10, respectively.

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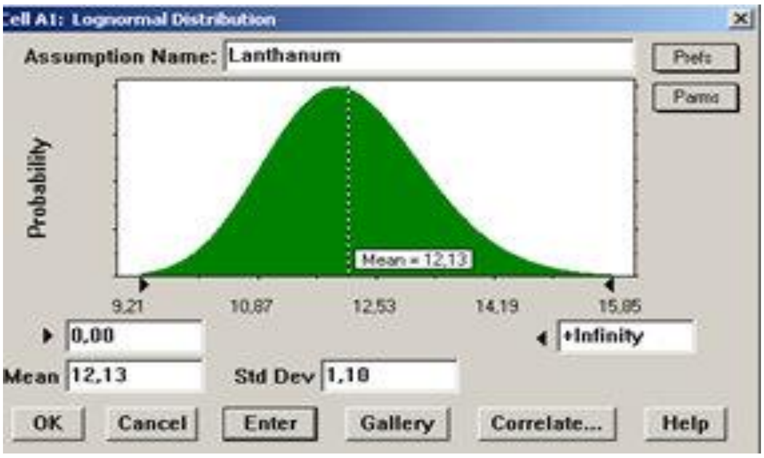


Assumption Name: Lanthanum

0,00

+Infinity

Mean 12,13

Std Dev 1,18

Fig. 2. The dialog windows of log-normal probability distribution of La, as obtained in CB software *(source: own work).*

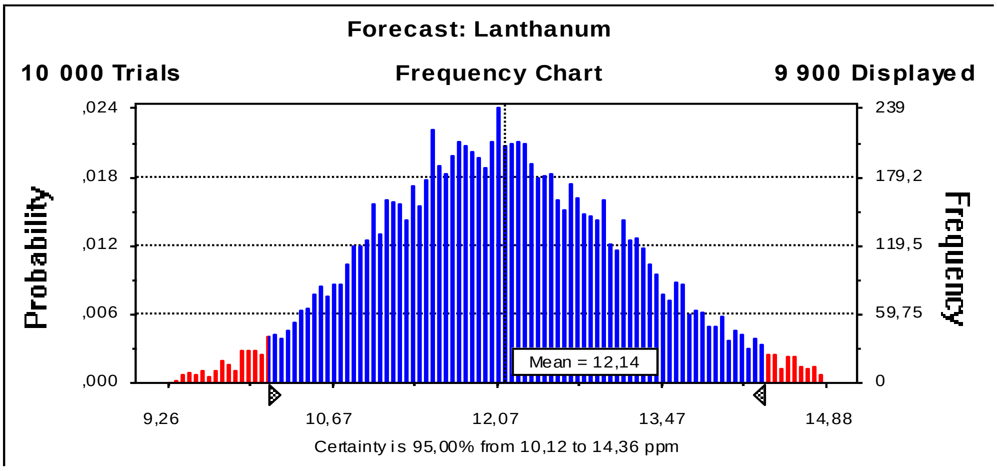


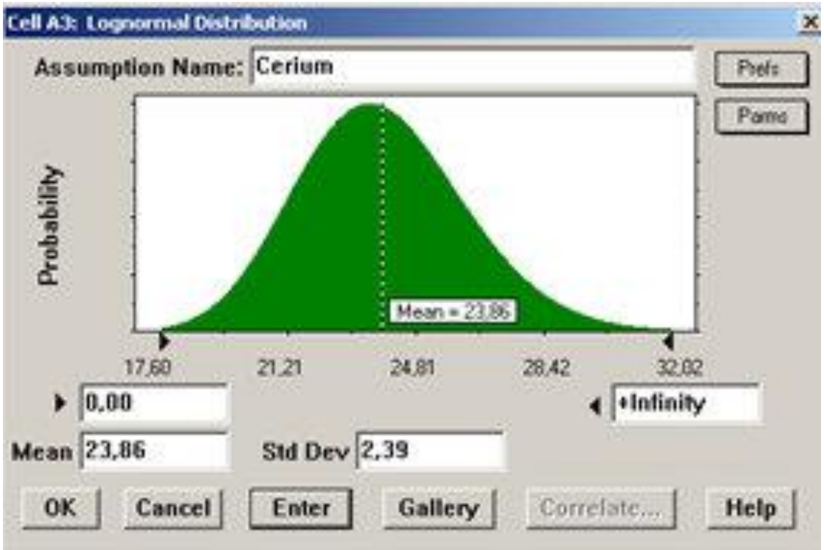
Fig. 3. The Frequency chart of the La forecast with 95% confidence level *(source: own work).*

Statistic	La (ppm)
Trials	10 000
Mean	12.14
Median	12.10
Mode	---
Standard deviation	1.09
Variance	1.19
Skewness	0.24
Kurtosis	3.14
Coeff. of variability	0.09
Range maximum	8.09
Range minimum	18.46
Range width	10.37
Mean std. error	0.01

Fig. 4. The statistics report of the forecast of the La – Statistics *(source: own work).*

Percentile	La (ppm)
0%	8.09
10%	10.78
20%	11.21
30%	11.55
40%	11.82
50%	12.10
60%	12.37
70%	12.69
80%	13.06
90%	13.58
100%	18.46

Fig. 5. The statistics report of the forecast of the La – Percentiles *(source: own work).*



Assumption Name: Cerium

0,00

+Infinity

Mean 23,86

Std Dev 2,39

Fig. 6. The dialog windows of log-normal probability distribution of Ce, offered in CB software *(source: own work).*

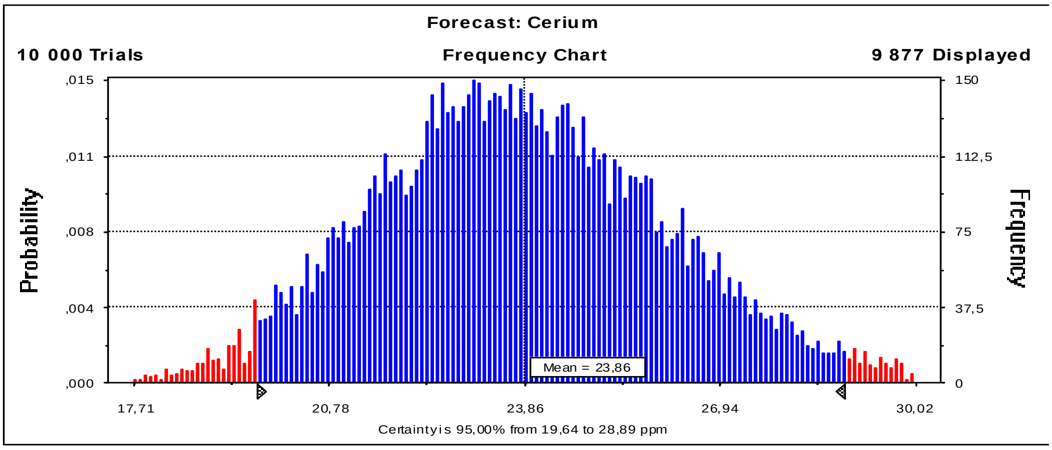


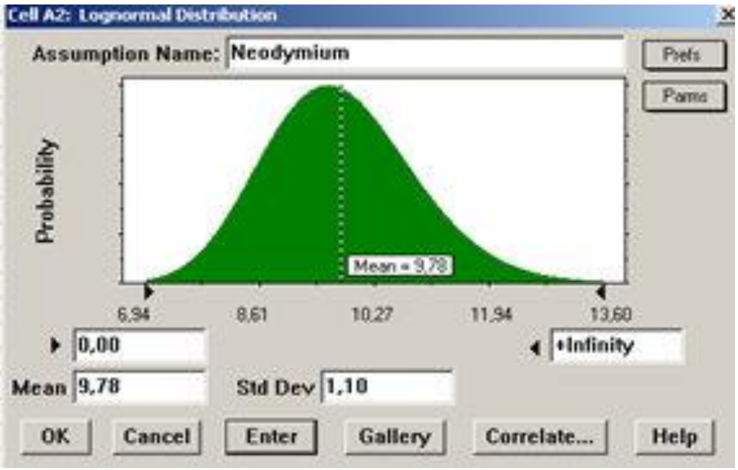
Fig. 7. The Frequency chart of the Ce forecast with 95% confidence level *(source: own work).*

Statistic	Ce (ppm)
Trials	10,000
Mean	23.86
Median	23.73
Mode	---
Standard deviation	2.37
Variance	5.61
Skewness	0.33
Kurtosis	3.20
Coeff. of variability	0.10
Range maximum	16.03
Range minimum	33.18
Range width	17.15
Mean std. error	0.02

Fig. 8. The statistics report of the forecast of the Ce – Statistics *(source: own work).*

Percentile	Ce (ppm)
0%	16.03
10%	20.91
20%	21.84
30%	22.56
40%	23.14
50%	23.73
60%	24.34
70%	25.00
80%	25.79
90%	26.93
100%	33.18

Fig. 9. The statistics report of the forecast of the Ce – Percentiles *(source: own work).*



Assumption Name: Neodymium

0,00

+Infinity

Mean 9,78

Std Dev 1,10

Fig. 10. The dialog windows of log-normal probability distribution of Ne,
offered in CB software *(source: own work).*

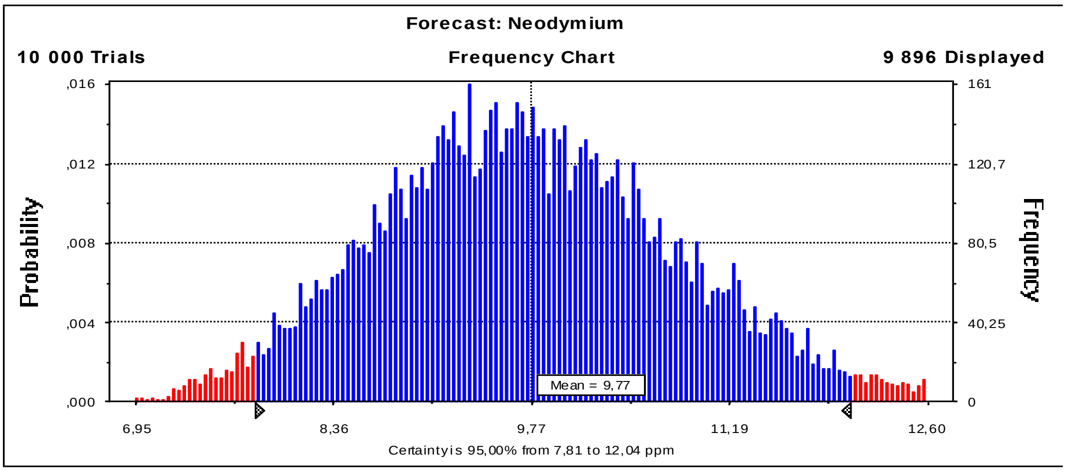


Fig. 11. The Frequency chart of the Nd forecast with 95% confidence level *(Source: own work).*

Statistic	Ne (ppm)
Trials	10 000
Mean	9.77
Median	9.72
Mode	---
Standard deviation	1.09
Variance	1.18
Skewness	0.34
Kurtosis	3.26
Coeff. of variability	0.11
Range maximum	6.47
Range minimum	16.71
Range width	10.24
Mean std. error	0.01

Fig. 12. The statistics report of the forecast of the Ne – Statistics *(source: own work).*

Percentile	Ne (ppm)
0%	6.47
10%	8.42
20%	8.85
30%	9.17
40%	9.45
50%	9.72
60%	9.99
70%	10.30
80%	10.66
90%	11.21
100%	16.71

Fig. 13. The statistics report of the forecast of the Ne – Percentiles *(source: own work).*

Tab. 1. Overview of the REEs taken into account in the study (all values in ppm).

REEs	Distribution type	Atomic number	μ_g	σ_g.	Quality	Reference
Lanthanum (La)	Lognormal	57	12.13	1.10	12.19	CB® analysis result
Cerium (Ce)	Lognormal	58	23.86	2.39	23.89	CB® nalysis result
Neodymium (Nd)	Lognormal	60	9.78	1.10	9.83	CB® analysis result

3. Results and discussions

MC simulation has received considerable attention in the literature, especially when MC simulation is used for making decisions that will have a large social and economic impact [20]. This is best seen in [21-26]. Di Maria et al. [14] proposed novel approach for quantifying uncertainty propagation in LCA and recommended MC simulation for carrying out an uncertainty analysis in LCA studies.

Bieda and Grzesik [23] provided definition of the uncertainty in the Article 3(6) of the Monitoring and Reporting Regulation - Guidance on Uncertainty Assessment No. 4, Final Version of 5 October 2012, part of a series of documents provided by the Commission services for supporting the implementation of Commission Regulation (EU) No. 601/2012 of 21 June 2012 (on the monitoring and reporting of greenhouse gas emissions pursuant to Directive 2003/87/EC of the European parliament and of the Council).

In the current study uncertainty analysis at the LCI level is conducted using Oracle Crystal Ball® (CB) associated with Excel spreadsheet models for carrying MC simulation. LCI data was defined as probability distributions instead of deterministic values.

The confidence interval is 95%. The total forecast value ranges of Ce, La, and Ne forecast value amounted to the mean values of 23.86 ppm, 12.13 ppm, and 9.78 ppm, respectively. The range centered about the mean from 19.64 ppm to 28.89 ppm for Ce, from 10.12 ppm to 14.36 ppm for La, and from 7.81 ppm to 12.04 ppm for Ne, respectively. Just below the horizontal axis at the extremes of distribution there are two small triangles, called endpoint grabbers. The confidence limits, presented in the frequency charts, are fixed using the above-mentioned grabbers (the area of the frequency charts covered by them is darker) [25].

4. Conclusions

This study aimed to express application of the stochastic approach to the neodymium, cerium and lanthanum, extracted from secondary sources of the REEs, classified as waste, and obtained during gold processing. The study also hope to promote the use of uncertainty analysis in environmental science based on the use of MC simulation. Furthermore, the goal of this study was to provide LCI data which can be further treated and used to the full LCA analysis of REEs recovery processes from secondary sources.

Under real conditions, primary data parameters are usually loaded with uncertainty. The uncertainty analysis for stochastic simulation requires that all parameters are described by probability distributions. In order to assess the credibility of the LCA results, which are burdened with a certain degree of uncertainty, the stochastic analysis, using the MC simulation has been adopted with the aim of evaluating the uncertainty in LCA.

This study combines the knowledge and insights from previous works about modelling of recycling with environmental data for REEs and continue to evaluate and discuss focus on the usefulness of stochastic modelling concerning uncertainty in the environmental engineering. This study also highlights the needs for further studies of REEs recovery. Presented study could be helpful in explaining the problems of stochastic analysis to scientific researchers, and to industry managers.

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