Application of stochastic approach based on Monte Carlo (MC) simulation for life cycle inventory (LCI) of the rare earth elements (REEs) in beneficiation rare earth waste from the gold processing: case study

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Abstract. The study proposes an stochastic approach based on Monte Carlo (MC) simulation for life cycle assessment (LCA) method limited to life cycle inventory (LCI) study for rare earth elements (REEs) recovery from the secondary materials processes production applied to the New Krankberg Mine in Sweden. The MC method is recognizes as an important tool in science and can be considered the most effective quantification approach for uncertainties. The use of stochastic approach helps to characterize the uncertainties better than deterministic method. Uncertainty of data can be expressed through a definition of probability distribution of that data (e.g. through standard deviation or variance). The data used in this study are obtained from: (*i*) site-specific measured or calculated data, (*ii*) values based on literature, (*iii*) the ecoinvent process „*rare earth concentrate, 70% REO, from bastnäsite, at beneficiation*". Environmental emissions (e.g, particulates, uranium-238, thorium-232), energy and REE (La, Ce, Nd, Pr, Sm, Dy, Eu, Tb, Y, Sc, Yb, Lu, Tm, Y, Gd) have been inventoried. The study is based on a reference case for the year 2016. The combination of MC analysis with sensitivity analysis is the best solution for quantified the uncertainty in the LCI/LCA. The reliability of LCA results may be uncertain, to a certain degree, but this uncertainty can be noticed with the help of MC method.

1 Introduction

All of the REEs, were finally identified in the 20th century. Promethium (Pm), the rarest, was not identified until 1945, and pure lutetium (Lu) was not refined until 1953 ([1–2]). Detailed history of REE production is presented in Castor and Hedrick [3].

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Rare-earth elements (REEs) are a group of 17 elements with similar chemical properties, including 15 in the lanthanide group, yttrium, and scandium because of their similar physical and chemical properties [2]. For more than two decades, at least 95% of annual global supply of the rare-earth elements (REEs) has been provided by Chinese rare-earth producers. Mining companies are now actively seeking for new exploitable rare-earth deposits, white old mines ae being reopened [4]. Life cycle assessment (LCA) takes a holitic approach and provides a complete view of the environmental impacts over the entire life cycle of a proces or product, from raw material extraction and aquisition, manufacturing, transportation and didtribution, use and maintenance, reuse and recycle, and all the way to disposal and waste management [2, 5, 7].

2 LCI data quality analysis

2.1 Data preparation

The LCI is a critical component as it is the data foundation of the LCA study [2]. The approach adopted by ISO 14040 is to compile the inventory based on the inputs and outputs fromeach of the processes (referred to as unit processes) involved in a product's life cycle [2, 8, 9].

An LCI analysis usually requires a large amount of data. The uncertainty of these parameters directly affects the outcome of any environmental impact method [10]. The overall uncertainty of an LCI is usually dominated by a few major uncertainties [11]. The use of stochastic model helps to characterize the uncertainties better than a purely analytical mathematical approach.

The aim of this study were to develop a stochastic approach for LCA technique limited to LCI uncertainty assessment for study for rare earth elements (REEs) recovery from the secondary materials processes production applied to the New Krankberg Mine in Sweden.

2.2 Uncertainty analysis of LCI

At the LCI level, Monte Carlo (MC) simulation was used. Stochastic nature of the MC method is based on random numbers [12–13]. The uncertainty, at LCI level, introduced into inventory due to the cumulative effects of input uncertainty and variability of inventory data was qualified by using expert judgment-based approach [14]. Uncertainty carried out in this study lead to a transparent increase in confidence in the life cycle impact assessment (LCIA), and finally LCA findings [14]. The complexity of many practical situations often requires simulation [15]. The MC method is recognized as an important tool in science [16]. MC simulation uses distributions to generate realistic random values. The benefits of simulation modeling approach are: (*1*) understanding of the probability of specific outcomes, (*2*) ability to pinpoint and test the driving variables within a model, (*3*) a far more flexible model; and (*4*) clear summary charts and reports [10]. In this work the MC sampling was carried out using an Excel® spreadsheet and Crystal Ball®, a software package which generates random numbers for a probability distribution. A large number of trials is required to obtain accurate results. The MC analysis-simulation is the only acceptable approach for U.S. Environmental Protection Agency (EPA) risk assessments [17]. Simulation models are generally easier to understand than many analytical approaches [15]. Bieda [13] quoted definition of the uncertainty presented in the Commission Decision of 18 July 2007 guidelines for the monitoring and reporting of greenhouse gas emissions pursuant to Directive 2003/87/EC of the European parliament and of the Council. Definition is defined as follow : "*a parameter associated with the result of the*

determination of a quantity that characterizes the dispersion of the values that could reasonably be attributed to the particular quantity, including the effects of systematic as well as of random factors and expressed in per cent and describes a confidence interval around the mean value comprising 95 % of inferred values taking into account any asymmetry of the distribution of values" [13].

2.3 Results

Data used in the study has been obtained from the following sources:
• site-specific measured or calculated data - the secondary materials processes production applied to the New Krankberg Mine in Sweden
• value based on information in the literature
• the ecoinvent process „*rare earth concentrate, 70% REO, from bastnäsite, at beneficiation.*

In the present study we discuss and modeled our LCI based on the proposed process for the beneficiation of REE in the flotation tailings from new Kankberg mine [18].

After the flotation stage, the concentrate that contains a mix of phosphates (apatite and monazite) can be further enriched through magnetic separation thanks to the paramagnetic property of monazite (apatite is non-magnetic) [18]. Magnetic separation leads to the production of a concentrate containing phosphate (P_2O_5) content (monazite mainly), cerium(Ce), lanthanum (La) and neodymium (Nd) [18]. The simulation results after 10,000 trials have been presented in the form of frequency forecast charts (Figs. 1, 2, 3 and 4), and and statistic reports (Tab. 1). The confidence interval is 95%. The total forecast value ranges of Ce, La, Ne and P_2O_5 forecast value amounted to the mean values of 170.02 ppm, 89.78 ppm, 70.00 ppm and 0.70%, respectively, ranging from 136.98 ppm to 203.37 ppm (see Fig. 1), from 72.06 ppm to 107.19 ppm (see Fig. 2), from 56.58 ppm to 83.76 ppm (see Fig. 3), and from 0.14% to 0.20% (see Fig. 4), respectively. The frequency chart is a histogram of the outcome variable that includes all values within 2.6 standard deviations from the mean, which represents approximately 99% of the data [15]. 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 above-mentioned grabbers (the area of the frequency charts covered by them is darker) [15].
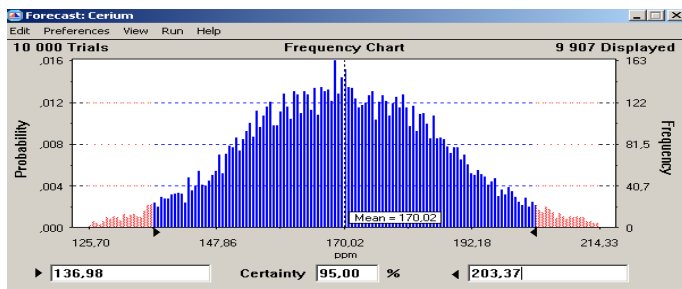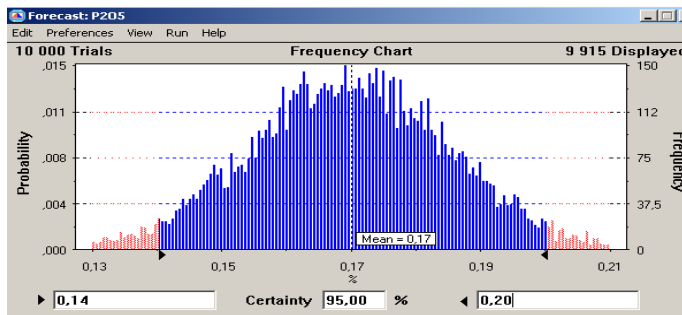

Fig. 1. Forecast frequency chart: Cerium (95% confidence level).
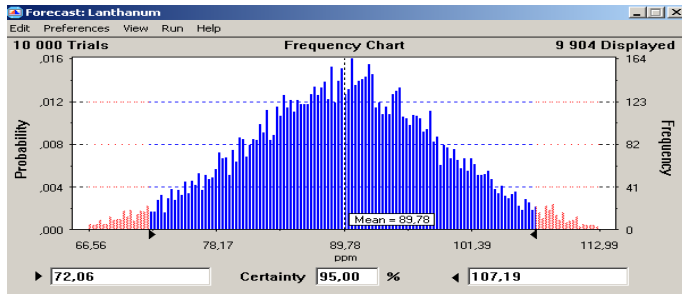
Fig. 2. Forecast frequency chart: Lanthanum (95% confidence level).
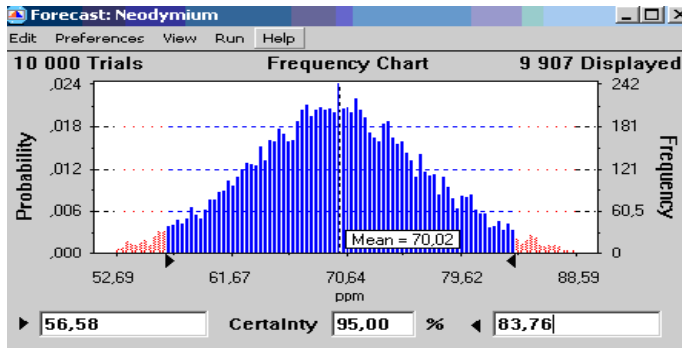
Fig. 3. Forecast frequency chart: Neodymium (95% confidence level).

Fig. 4. Forecast frequency chart: P_2O_5 (95% confidence level).

Table 1. Statistics of outcomes from the simulation (Ce, Ne, La, P_2O_5)

3 Conclusions

The aim of the study was to using a stochastic modelling based on the MC simulation for LCI to the rare earth elements (REEs) in beneficiation rare earth waste from the gold processing: case study, as well as to promote the use of uncertainty approach in environmental science. Uncertainty analysis in the LCA methodology has received increasing attention over the last years.

The use of MC simulation allows for saving in time and resources. Application of the MC simulation into the LCA of the production of rare earths, may give support in the interpretation of LCA results and permit to better understanding of many analytical approaches. Generally, in a deterministic model, all data is known, while in a probabilistic model, data is presented and described by probabilistic distributions. LCA/LCI data is full of uncertain numbers, and the MC analysis is a useful approach of quantifying parameter uncertainty in LCA studies.

Thanks to uncertainty analysis, a final result is obtained in the form of value range. The results obtained from this work can help practitioners and decision makers in the environmental engineering. Lack of uncertainty analysis in LCI has influence on the LCIA results, and finally on the LCA outcomes.

The results of the study were the base for decision making process. Moreover, these results move the LCI study on the rare earth elements (REEs) recovery from the secondary materials processes production one step forward.

Recommendations and outlook

The research described in this paper can also serve as the basis for future scientific work. The potential direction for future research is to integrate LCA and risk assessment for industrial processes. A complementary paper about LCIA will be produced.

Acknowledgments

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