Environmental Impact Assessment Review 73 (2018) 122–127

Contents lists available at ScienceDirect

Environmental Impact Assessment Review

journal homepage: www.elsevier.com/locate/eiar

Multi-criteria ranking of chemicals for toxicological impact assessments

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1. Introduction

The global regulatory and societal trend of environmental awareness is strongly pushing companies to incorporate environmental sustainability into their business models. The adoption of environmental management systems (EMS) such as ISO 14001 can encompass compliance with regulatory requirements. However, growing ethical reasoning in customers' decision is motivating companies to go further in developing environmental programs extended to their supply chain, and disseminating them through the publication of up-to-date sustainability reports. The release of toxic substances from manufacturing plants and finished products are among the key variables to be included in an effective EMS. In order to set up efficient monitoring programs and corrective actions, priority chemicals must be identified based on their toxicological relevance. Still, toxicity data of a chemical substance may refer to a variety of exposure routes (e.g. inhalation, ingestion, dermal contact etc.) and effects (e.g. reversible injuries, acute or chronic lethality, carcinogenicity, etc.), which are not directly comparable. For this reason, toxicity evaluations are currently carried out by following risk assessment strategies based on single types of hazard or exposure route. The US Environmental Protection Agency (EPA) (2009) adopted this approach, providing a risk assessment guidance for the independent evaluation of carcinogenic and non carcinogenic inhalation risks, by comparing the exposure concentration to distinct reference values (the inhalation unit risk and the hazard quotient, respectively). However, this approach does not allow to obtain an univocal ranking of global toxicity. Some attempts have been made in this direction. For instance, a Safer Chemical Ingredient List was created by US EPA (2016) with the aim of help consumers in finding products that perform well and are safer for human health and the environment. Within this list, increasingly safer alternatives of commercial ingredients are marked with a yellow triangle, a green half-circle or a green circle. A similar classification is given by GreenScreen® For Safer Chemicals (Clean Production Action 2016), which sets out 4 benchmarks that define progressively safer chemicals. In both cases, the limited number of categories used for classification of chemicals may smooth down significant differences in toxicity among chemical compounds. In Europe REACH (Registration, Evaluation, Authorisation and Restriction of Chemicals), the new regulation regarding the production and use of chemical substances, addresses in particular companies that may play a role as manufacturer, importers or downstream users. REACH defined a "List of restricted substances", constituted of substances that cannot be used in the specified restriction conditions (European Chemical Agency (ECHA), 2018). Moreover, it introduced a procedure for the identification of the "Substances of Very High Concern" (SVHC), that are candidates for substitution. REACH SVHC criteria are severe hazardous properties such as carcinogenic, mutagenic, toxic for reproduction (Berges et al., 2014). REACH and the other resources could be a good starting point for companies that need to set-up corrective actions, but none of these classification methods permits to obtained a detailed order of priority to be given to substances for their replacement.

In this work, a novel approach for toxicological ranking of chemicals has been developed by designing a dedicated multi-criteria method. Multi-criteria analysis (MCA) is a family of decision-making tools that are mostly used in strategic environmental assessment procedures to ensure that environmental, societal and economic variables are all taken into consideration within (Convertino et al. 2013; Omo-Irabor et al. 2011; Srivastava et al. 2012; Valle Junior et al. 2015). All variables are integrated to extract a synthetic aggregated value for each case to be compared (e.g. each geographical region or intervention scenario). The aggregated values are then categorised based on evaluation criteria which represent utility values for the stakeholders, and finally ranked. The MCA approach has been successfully implemented in the fields of energy planning (Pohekar and Ramachandran 2004), agriculture (Hayashi 2000), water resource management (Hajkowicz and Collins 2007), and many others, but to our knowledge, has never been used with the aim of evaluating the global toxicity of chemicals in any kind of samples.

In this work, MCA was adapted to create a ranking strategy for chemicals by combining their hazard for humans and the environment, with the measured concentration in cases of interest (manufacturing plants, products, geographical regions etc.). The method goes beyond classical toxicological evaluations, based on a single and specific type of toxicity, because MCA can take into consideration a potentially unlimited number of parameters at the same time, leading to a ranking of compounds based on a global hazard concept. Since every criterion could be assigned a relative weight, the method leads to the

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https://doi.org/10.1016/j.eiar.2018.08.001
Received 29 March 2018; Received in revised form 2 August 2018; Accepted 3 August 2018

construction of a dynamic ranking of compounds (or general scenarios) that may be updated at any change of the input values (measured concentration of chemicals) and relative importance of criteria. This feature makes the proposed MCA approach very versatile and applicable to a wide variety of fields. Two case studies are presented, focused on the textile sector, where MCA was implemented to evaluate: i) the chemical-toxicological impact of manufacturing facilities through wastewater effluents; ii) the direct impact of the pollutants' content in consumer goods (clothing). Despite available data were insufficient to achieve a complete overview of the impact of textile industry worldwide; they provide a representative view of method applicability, to be intended in combined use with classical statistical techniques. The method is of simple implementation, as it does not require experimental phases; reliable, because toxicological data are official and provided by universally recognised agencies; and versatile, as it can be used for environmental evaluations in various fields, and for different purposes.

2. Material and methods

2.1. Chemicals

Globally, 240 different chemical compounds of toxicological relevance were selected for the comparison. They belong to a wide variety of classes, including: alkylphenols, phthalates, flame retardants, dyes, organotin compounds, poly- and per-fluorinated substances (PFAS), chlorobenzenes, chlorotoluenes, solvents, phenols, short-chain chlorinated paraffins, metals and metalloids, cyanide, pesticides, biocides, organic phosphor acetic acid esters, volatile organic compounds (VOCs, − including polycyclic aromatic hydrocarbons (PAHs) - and diisocyanates. The complete list of chemicals is reported in the Supplementary Material (Table S.1).

2.2. Concentration data and samples

Data for the implementation of the case studies is constituted of a real set of concentration values, provided by a multinational corporation in the textile sector. Water sampling has been performed over four years (from 2013 to 2016) at 15 manufacturing facilities, located in 7 countries (China, Bangladesh, Turkey, Portugal, Italy, Croatia and Egypt), for a total of 17 wastewater samples. Clothing is represented by a set of 16 samples, all collected in 2017. Since concentration data are used only as a demonstration of the application of the described method, analytical details (analytical methods, quality controls, etc) are not reported herein. Due to business secrecy, further information about the wastewater sampling sites and clothing specifications are not provided.

2.3. Data elaboration

Comparing compounds characterised by different kinds of toxicity is not a trivial task. For instance, must be acute toxicity considered more relevant than carcinogenicity? Should be an endocrine disruptor considered more significant than a compound toxic for the aquatic ecosystem? Clearly, defining the relative importance of different toxicity indexes must be the first step of the analysis. It must be also taken into account that some compounds can be associated to different types and values of toxicity at the same time. MCA is typically used to evaluate project priorities as the alternative scenarios, thereby enabling project managers to make comprehensive and well-informed decisions. In such context, criteria could potentially include environmental, societal and economic aspects. In this work, MCA was applied by choosing chemical compounds as the alternative scenarios, and different kinds of toxicity as criteria. The subsequent elaboration proceeded according to the following steps, outlined in the next paragraphs: i) identification and selection of criteria (toxicity indexes); ii) definition of performance measures (toxicity level) for each alternative (chemical); iii) transformation of the performance measures into commensurate units; iv) calculation of the criteria relative weight; v) calculation of global toxicity score for the alternatives (chemicals); vi) calculation of global toxicity score for the samples (wastewaters and garments).

2.3.1. Identification and selection of criteria (toxicity indexes)

In order to conduct a global toxicological evaluation, various kinds of toxicity were identified as criteria. Specifically, health and environmental hazards, as classified within the "Globally Harmonized System of classification and labelling of chemicals" - GHS (United Nations 2013), were selected. Health toxicity was represented by acute toxicity (AT), skin corrosion/irritation (SC), serious eye damage/eye irritation (SED), respiratory sensitization (RS), skin sensitization (SS), germ cell mutagenicity (GCM), carcinogenicity (CAR), reproductive toxicity (RT), specific target organ toxicity (STOT), the latter being measured by single exposure (STOT-s) or repeated exposure (STOT-r), and aspiration hazard (AH). Acute toxicity was also classified on basis of the exposure route: oral (AT-o), inhalation (AT-i) and dermal (AT-d). Environmental hazards were represented by the hazard to the aquatic environment (HAE), measured as acute toxicity (HAE-AT) and chronic toxicity (HAE-CT), and hazard to the ozone layer (HOL). Within GHS, the levels of toxicity are expressed by categories, where category 1 is always the maximum level of hazard.

2.3.2. Definition of performance measures (toxicity level)

At this stage, the decision-maker usually selects a score from a range of values that expresses the performance of each criterion for all alternatives. Here, the level of toxicity, represented by the categories of hazard, was identified as the performance measure of each chemical in terms of toxicity. Each category was converted into a toxicological equivalent value (TEV) ranging from 0 (no toxicity) to 1 (maximum toxicity), as shown in Table 1.

2.3.3. Calculation of criteria relative weight

In MCA, relative weights can be determined by pair-wise comparison, a mathematical technique that quantifies the relative weights of criteria by dividing the complex decision problem into a series of one-to-one judgements about the significance of each criterion relative to the others (Garfì et al. 2011). For each pair-wise comparison, a value from 1/9 (extremely less important) to 9 (extremely more important) was assigned, 1 being representative of equally important criteria. The comparison values were collected into a square matrix, where the

Table 1
Toxicological equivalent values (TEVs).

AT-o		AT-i		AT-d		SC		SED	
CAT 1	1000	CAT 1	1000	CAT 1	1000	CAT 1/1A	1000	CAT 1	1000
CAT 2	100	CAT 2	100	CAT 2	100	CAT 1B	50	CAT 2/2A	1
CAT 3	5	CAT 3	20	CAT 3	20	CAT 1C	20	CAT 2B	0.1
CAT 4	1	CAT 4	5	CAT 4	5	CAT 2	1		
CAT 5	0.2	CAT 5	2			CAT 3	0.1		
RS/SS		GCM/CAR		RT		STOT-s		STOT-r/AH	
CAT 1/1A	1000	CAT 1/1A	1000	CAT 1/1A	1000	CAT 1	1000	CAT 1	1000
CAT 1B	100	CAT 1B	100	CAT 1B	100	CAT 2	100	CAT 2	1
		CAT 2	1	CAT 2	1	CAT 3	1		
				EL*	0.1	CAT 4	0.1		
HAE		HOL							
CAT 1	1000	CAT 1	1000						
CAT 2	100								
CAT 3	10								
CAT 4	1								

EL*: Effect on or via lactation.