Hazard and Life Cycle Assessment of Safe and Sustainable Coatings

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Abstract. The PROPLANET project develops innovative bio-based coatings for textiles, food packaging machinery, and glass implementing a Safe and Sustainable by design (SSbD) approach to replace per- and polyfluoroalkyl substances (PFAS) compounds. A hazard assessment approach is carried out integrating a detailed toxicological *in vitro* assessment. Key toxicological endpoints, including cytotoxicity, genotoxicity, and pro-inflammatory responses are analysed in the chemicals formulations that replace PFAS-based coatings to ensure human health safety. Additionally, a Life Cycle Assessment (LCA) is conducted to evaluate the environmental impact of these formulations. Combining hazard assessment and LCA criteria enables the development and optimisation of coatings with low health and environmental risks. Furthermore, these assessments support PROPLANET's PFAS-free coatings in meeting regulatory requirements and market demands by promoting safe, efficient, and eco-friendly solutions for industrial applications. The integration of these methodologies strengthens the transition toward safe and sustainable materials and products in a circular economy framework.

Keywords: Safety · Sustainability · PFAS · LCA · coatings

1 Introduction

Per- and polyfluoroalkyl substances (PFAS) are widely used in coatings due to their excellent durability, water repellence, and resistance to chemicals [1]. Despite these advantages, PFAS have become a major environmental concern because of their persistent nature and potential to bioaccumulate, posing significant risks to ecosystems and human health [2]. Recent regulations have increased pressure on industries to find safer alternatives, leading to the exploration of alternative chemical formulations for coatings [3].

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Assessment of environmental and health risks associated with alternative formulations requires robust analytical methodologies such as hazard assessment and environmental life cycle assessment (LCA) [4, 5]. Hazard assessment identifies and characterises the inherent toxicity, persistence, and bioaccumulation posed by chemicals, considering factors such as toxicity, persistence, and bioaccumulation potential [6]. Meanwhile, environmental LCA provides a comprehensive evaluation of environmental impacts associated with all stages of a coating's life cycle, from raw material extraction to final disposal [7].

The differences between risk assessment and LCA are a matter of perspective, as the former focuses on evaluating and managing a toxicological hazard within a defined exposure scenario, while the latter aims at a comprehensive evaluation of the impacts of numerous substances across various media, including non-toxicological effects. Hence, risk assessment mainly focuses on receptors (i.e. humans and environment), while LCA focuses on emitters [8]. Combining these approaches enables a thorough assessment and facilitates informed decision-making towards safer and more sustainable alternatives [9].

Such integration is critical essential in product development processes, as it aligns industrial practices with emerging regulatory frameworks and sustainability objectives. It has been previously suggested that integration of risk assessment and LCA at the level of results, rather than along the methods, could be a more pragmatic approach. Therefore, the aim of this article is to present a methodology for integration of hazard assessment and LCA results and ranking alternative coating formulations based on their impact on their toxicity and the environment. This methodology was applied to the textile case study of the PROPLANET project, to replace PFAS in new coatings.

2 Materials and Methods

The formulations under assessment consisted of four PFAS-free chemicals mixtures, based on natural biopolymers, such as polysaccharides and waxes. The samples are coded A-D and developed by the National Institute of Chemistry, Department of catalysis and chemical reaction engineering (NIC). The coatings formulations were developed as part of the PROPLANET project, and its manufacturing process is protected by the project's intellectual property. To choose which formulation developed as an alternative to PFAS is the safest and most sustainable, hazard assessment and LCA were carried out and the results aggregated.

2.1 Hazard Assessment

Four liquid-form water-based test substances were labelled as: A, B, C, D. Hazard assessment was performed through *in vitro* studies on the human alveolar cell line A549. The endpoints investigated were cytotoxicity (reduction of cell viability) through the Alamar Blue assay, genotoxicity (DNA damage) through the Comet assay, and the release of the pro-inflammatory mediator interleukin (IL)-6 through the Enzyme-Linked Immunosorbent Assay (ELISA). Briefly, the cells were maintained in DMEM medium supplemented with 10% FBS and 1% penicillin/streptomycin, in an incubator with humidified atmosphere at 37 °C, 5% CO_2. The test substances were mixed with cell culture medium

immediately before exposure at concentrations ranging from 0.01 to 5% (v/v). After 24 h exposure, the cells were processed for further analyses as previously described (Alamar Blue: Longhin et al. [10]; Comet assay: El Yamani et al. [11], ELISA by Thermo Fisher Scientific was run according to the manufacturer's instructions). For all the assays, three independent experiments were run (biological replicates), with two technical replicates run in each independent experiment.

Based on the results obtained in the assays, toxicity scores were assigned for each of the investigated endpoints. For cytotoxicity, a scoring scheme was adapted from El Yamani et al. [12]. As described in Table 1, the approach assigns score points based on the level of toxicity and half maximal Effective Concentration (EC50) reached. For example, a test substance induced cytotoxicity by 60% with respect to Negative Control (NC), and had EC50 at the exposure concentration of 2%, would be assigned 2 points for the intensity of the effect reached (toxicity reaches 20% $\rightarrow$ assign $+$ 1 point AND toxicity reaches 50% $\rightarrow$ assign another $+$ 1 point $=$ total 2 points), and 4 points for the EC50 (EC50 $<$ 5% $\rightarrow$ $+2$ AND EC50 $<$ 2.5% $\rightarrow$ $+2$), for a total of 6 points. A similar system was here developed for the release of pro-inflammatory mediator IL-6, with the difference of using the lowest observed effect concentration (LOEC) as parameter instead of EC50 (see Table 1).

Table 1. Hazard scoring scheme for cytotoxicity and pro-inflammatory response (IL-6) of PROPLANET's test substances. EC50: concentration that gives half of the maximal response. LOEC: lowest observed effect concentration. NC: negative control.

	Toxicity reaches - % represents increase over NC			EC50 (cytotoxicity)/LOEC (IL-6) – % represents test substance concentration		
Cytotoxicity	20%	50%	80%	<5%	<2.5%	<1%
IL-6	50%	100%	200%	<5%	<2.5%	<1%
Score Points	+1	+1	+1	+2	+2	+2

For genotoxicity, the test substances were categorized as positive, negative, or equivocal based on the criteria described in El Yamani et al. [12]. Briefly, substances are classified as positive if at least two tested concentrations are statistically significantly different from the NC level (by One-way ANOVA), or at least one concentration is different "AND" there is a significant linear trend (by simple linear regression analysis). The category equivocal is assigned in case there is a significant linear trend "OR" one concentration significantly different from NC. A substance is classified as negative if none of the criteria above are met, i.e. the level of effect is similar to the NC.

Based on the results obtained, a hazard score and category were assigned to each endpoint according to Table 2. The system was adapted from El Yamani et al. [12], to align with JRC's approach [13], where a high score indicates safer alternatives. In this case, non-toxic formulations receive a score 3, and toxic formulations receive a score of 1. The endpoints were then weighted according to their severity. Cytotoxicity and pro-inflammatory response were assigned a weight of 0.25 each, while genotoxicity was assigned a weight of 0.5 (total weight $=$ 1). The hazard score for each the endpoint was

multiplied by its assigned weight, and the endpoints scores were summed to obtain an overall hazard score.

Table 2. Hazard category and score applied for the ranking of the test substances, based on the single assays scores.

Hazard category	Hazard score	Cytotoxicity/IL-6 score	Genotoxicity score
Toxic	1	6–9	Positive
Slightly toxic	2	2–5	Equivocal
Non-toxic	3	0–1	Negative

In the example on cytotoxicity presented above, where the test substance is assigned a cytotoxicity score of 6, this corresponds to a hazard score of 1, and thus a cytotoxicity weighted score of 0.25. This will be combined with the IL-6 and genotoxicity weighted scores to determine the overall hazard score.

2.2 Life Cycle Assessment

The methodology proposed in ISO 14040/44 was followed to obtain the results through the four steps 1) 'Goal and scope', 2) 'Life cycle inventory', 3) 'Life cycle assessment' and 4) 'Interpretation'. 1) The aim of this evaluation is to compare the environmental impacts of the developed coating formulations as PFAS alternatives. The boundary used to determine the scope of the assessment was 'cradle to gate', regarding the formulation of the coating. The functional unit used was 1 kg of coating produced. 2) The life cycle inventory contains the information flow of matter used in the processes included in the boundary, these were provided by the coating formulations developer (NIC, a PROPLANET partner). 3) The assessment was carried out with SIMAPRO v9.0 software, using the ReCiPe method [14] to characterise the end-point impact categories. 4) The results were interpreted to rank the results according to the environmental impacts caused by each formulation. Normalisation is carried out by multiplying the characterisation results by the inverse of the annual *per capita* reference values. This mathematical approach helps to identify which impacts are more significant than others.

2.3 Results Integration

To effectively integrate hazard assessment and LCA, it was firstly established that it should occur at the results level rather than the methods level. This is due to the fundamentally different objectives, boundaries, and data requirements of each approach [8]. This approach aligns with a post-analysis method, in which techniques such as LCA and hazard assessment are performed separately, and their outcomes are later combined to guide decisions (either through qualitative judgement or quantitative measures) [15]. In this context, the resulting ranking is based on the combined health and environmental impact of the formulations, that were identified through hazard assessment and LCA carried out in this study.

3 Results

3.1 Hazard Assessment

The cytotoxic potential of the formulations was tested on A549 cells at concentrations from 0.01 to 5% by the Alamar Blue assay. After 24 h exposure, the test substances exhibited different degrees of cytotoxicity. In particular, the formulations B and C were non-cytotoxic at the concentrations tested, while A and D induced almost complete cell death at the highest tested concentration (maximum cytotoxicity 99.3 and 97.9% respectively). The EC50 was 0.98 and 2.4% respectively for the test substances A and D.

Non- or slightly cytotoxic concentrations (cytotoxicity < 40%) were selected to further investigate the other endpoints, pro-inflammatory potential, and genotoxicity. The formulation C was the only one showing a slight release of the inflammatory marker IL-6 (70.9% over NC) with a LOEC of 2.5%. No release of IL-6 was observed with the other formulations. Regarding genotoxicity, the formulations A and D presented a significant linear trend ($p < 0.01$), but none of the concentrations presented a statistically significant increase over the NC, thus they were classified as equivocal. Formulations B and C were negative for genotoxicity.

Based on the results obtained in the in vitro assay, the weighted endpoints scores are reported in Table 3, together with the overall hazard scores (i.e., the sum of the weighted endpoints scores), and hazard category. Formulation B had the best hazard score, followed by C. The test substances A and D showed the last favourable performance in terms of hazard potential.

Table 3. Endpoints weighted scores and overall hazard scores for the test substances analysed.

Substance	Cytotoxicity score	Inflammation score	Genotoxicity score	Hazard score	Hazard category
A	0.25	0.75	1	2	Slightly toxic
B	0.75	0.75	1.5	3	Non-toxic
C	0.75	0.5 (*0.75)	1.5	2.75	Slightly toxic
D	0.25	0.75	1	2	Slightly toxic

* So far, unlike genotoxicity, the scoring system for cytotoxicity and inflammation does not take the variability of the data into account. Considering the variability observed in the experiments at the basis of the scores reported, the Inflammation score of substance C (0.5) has a high level of uncertainty, and a score of 0.75 could be assign instead. Further experiments are ongoing to reduce the endpoint's uncertainty.

3.2 Life Cycle Assessment

The normalised end-point results of the ReCiPe method are shown in Fig. 1. The total shown represents the sum of the damage in each category (the higher the number, the

greater the impact of the formulation). The results show that formulation B has the lowest damage impacts in the categories assessed. It is therefore considered the best formulation option from an LCA perspective. In contrast, formulation A has the highest overall impact values and is considered the worst PFAS-free formulation alternative. These results are related to the composition of each formulation. Materials of natural origin, whether synthesised or oil-based, tend to have different impacts on the environment and its various sectors (such as health, resources, and the ecosystem). Formulations C and D are at an intermediate level and show a similar behaviour between the results obtained. Through adjustments, these could become viable options from an LCA perspective. The 'human health' category is the most relevant to this study, as shown in Fig. 1, with the highest impact values among the categories. Due to the variation between the formulations, it is possible to identify that the differences between them are reflected in the results of this category. Therefore, category is decisive for determining the best and worst options.

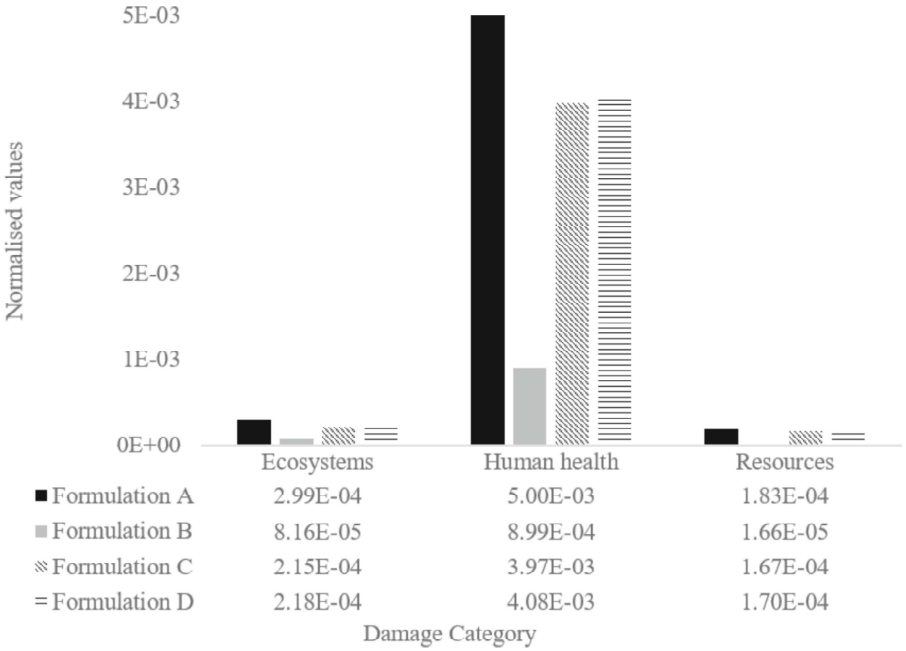

Fig. 1. Normalised end-point results of LCA using the ReCiPe method.

3.3 Integration Methodology

In this study, the integration was performed by expert judgement, based on the results obtained in the two dimensions: safety, as assessed by hazard assessment and sustainability as assessed by LCA. The integrated results of this study are presented in Table 4. Based on the assessments, formulation B is the safest and most sustainable of the four alternatives. The result of the integrated approach is also in line with the two dimensions, since this is the best performing formulation. Formulation C is the second-best

performing formulation in both dimensions. One of the strengths of this system is to allow innovators to make thoughtful decisions, weighting in both hazards and LCA. In this way, when two formulations are tied for one assessment, the other one can help deciding the best alternative. This occurred with formulations A and D, which had the same result for the hazard assessment, but formulation D performed better in the LCA. This suggests that formulation D may be a more suitable coating alternative. The LCA, revealed the greatest difference between formulations in the 'human health' impacts category at the endpoint assessment. This result supports the integration of methodologies, as it shows that the outcomes in this area (health) are distinct and warrant attention.

Table 4. Results of the formulations per assessment. The formulations are listed from the best to the worst performing according to the hazard assessment-LCA results integration.

Formulation	Hazard assessment results	LCA results
Formulation B	3	9.97E-04
Formulation C	2.75	4.35E-03
Formulation D	2	4.46E-03
Formulation A	2	5.48E-03

It is noteworthy that the results obtained in the LCA for the human health category align closely with the hazard assessment results. The LCA uses data on human and health impacts expressed in Disability-Adjusted Life Years (DALY), which are calculated from emissions and fate-exposure-effect modelling using the ReCiPe method. In contrast, the hazard assessment is derived from *in vitro* studies, as a model to investigate specific biological endpoints. Thus, these two methodologies address the "human health" aspect from different perspectives and approaches. The results similarity may be considered as a cross-validation of the methodologies and results, strengthening their credibility.

4 Conclusion

In recent years, concerns about PFAS in recent years have led to the creation of regulations aimed at eliminating their use in various sectors. The European project PROPLANET aims to develop safe and sustainable PFAS-free coatings. With the goal of aiding SSbD development, this work presented a methodology for integrating hazard assessment and LCA. The formulations developed for the textile case study in the PROPLANET project were used as a test case for applying the proposed methodology.

The evaluations were integrated using the results obtained individually in the hazard assessment and LCA. Both assessments revealed the same result, with the safest and most sustainable formulation being B and the least being A. At this stage, the integration was done qualitatively by expert judgment, based on the results obtained in the two dimensions. This was facilitated by the fact that the results from the hazard assessment and LCA were very much in line. In situations where the results differ between different dimensions, as possibly more dimensions are added (like socio-economic aspects), this

approach might be difficult to apply. As a further development, a quantitative approach for the integration might be explored, where different dimension scores are aggregated.

Future work could also address common characteristics between the impact and damage categories of risk assessments and LCA. Another possible line of research is the creation of more sensitive scores to distinguish the ranking position of each material assessed. The system here presented will be thus further refined through future activities in the PROPLANET project.

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