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Assessment of functional alternatives to fluorinated foam blowing agents in insulation materials

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Using the substitution of fluorinated gases employed as foam blowing agents in insulation materials as a case study, we aim to apply and adapt a well-established multi-criteria decision analysis (MCDA) method for chemical alternatives assessment, the multi-attribute utility theory (MAUT) approach, to evaluate and compare non-chemical alternatives based on technical performance and environmental impact attributes. The functional substitution approach was followed to define the functions delivered by fluorinated gases in insulation materials, and the ZeroPM alternatives database was used to identify functional alternatives. Data on environmental impacts along the life cycle, and the technical performance of the identified alternatives were collected based on previous literature reviews on insulation materials. The MAUT approach was used to compare the different alternatives. Four decision-making scenarios were defined in order to illustrate the flexibility of the MAUT method for the assessment of functional alternatives. Overall, 32 alternative materials to polyethene foams (also known as polyethylene foams) and extruded polystyrene foams containing fluorinated gases were identified. 9 insulation materials were shortlisted for further evaluation based on the amount of data available. Overall, alternatives ranked better than polyethene foams and extruded polystyrene foams in every decision-making scenario tested in this study, suggesting that suitable and safer alternatives to fluorinated gases used in insulation foams can be identified. This work highlights how the choices made by the decision-maker to develop a MAUT model influence the final ranking of the alternatives being evaluated. This might be highly relevant in a regulatory context as the availability of suitable alternatives is a critical part in the decision-making on bans of harmful substances. Although promising in the field of alternatives assessment in a regulatory context, further work is needed to develop appropriate guidance for using MAUT methods to identify suitable alternatives to substances of concern.

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Sustainability spotlight

When eliminating a substance of concern from processes or products, potential alternatives capable of providing similar functions should be carefully evaluated to prevent regrettable substitution. Although alternatives assessment frameworks have already been published, research is needed to ensure their proper implementation, especially when comparing alternatives which are not other chemical substances. Using the case of fluorinated gases employed as blowing agents in insulation foams, this study proposes a transparent method to ensure that decision-makers' preferences and requirements are made explicit during the evaluation of alternatives. This work contributes to the advancement of Sustainable Development Goals (SDGs) 9 (Industry, Innovation and Infrastructure), 11 (Sustainable Cities and Communities), and 12 (Responsible Consumption and Production).

1. Introduction

Regulations on uses of chemicals are in place worldwide in order to protect people and the environment from the risks posed by harmful chemicals. For instance, the Stockholm Convention is a global treaty which entered into force in 2004 with the aim of protecting human health and the environment from persistent organic pollutants (POP) through the restriction or elimination of the production and uses of such chemicals.[1] At the European level, the REACH Regulation (Registration, Evaluation, Authorisation and Restriction of Chemicals No. 1906/2006 EC)[2] entered into force in 2007 and aims to "ensure a high level of protection of human health and the environment […] while enhancing competitiveness of the EU chemicals industry".[3] Within REACH, the Restriction and Authorisation processes aim to restrict or ban in the EU uses of the substances presenting the greatest concern for human health and the environment.[4,5]

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Eliminating a substance of concern will typically mean some kind of alternative is needed. Careful evaluation of potential alternatives is needed to prevent "regrettable substitution" from occurring.[6,7] Regrettable substitution occurs when a substance is introduced to replace a chemical of concern, but the substance is then found to be of concern as well. For instance, hydrofluorocarbons (HFCs) were introduced as replacements to chlorofluorocarbons (CFCs) after the Montreal Protocol entered into force in 1989 to regulate ozone layer depleting substances.[8–10] In 2016, uses of some HFCs were later restricted following an amendment of the Montreal Protocol due to their high global warming potential (GWP).[8,11] Those substances were then replaced by other HFCs with lower GWP hydrofluoroolefins (HFOs) which have a significantly lower GWP than HFCs.[12,13] However, it has been demonstrated that several HFOs and HFCs can degrade in the atmosphere to form trifluoroacetic acid (TFA)[12,14] which is now under evaluation to be classified as toxic to reproduction; persistent, mobile and toxic (PMT); and very persistent and very mobile (vPvM)[15,16] in Europe.

To prevent regrettable substitution, methods for the assessment of alternatives to substances of concern have been developed.[7,17] In a nutshell, an alternatives assessment aims to identify, compare, and select safer alternatives to a chemical of concern (including alternative materials, processes and technologies) by considering their hazard profile, potential change in exposure, overall environmental impacts across the life cycle, technical performance, and economic viability.[5–7] The functional substitution approach was developed in order to help decision makers to identify all types of alternatives (*e.g.* alternative materials, products, technologies) to a substance of concern for a specific use.[18] In short, according to this approach the function of a substance should be defined on three different levels when defining the use of the substance of concern: the chemical function, which corresponds to the actual technical function delivered by a substance, generally defined by its physicochemical properties; the end-use function which describes the general properties a substance brings to the product or process according to its chemical function; and function as service which describes the benefits that a substance used in a specific product or process brings to society.[18] By focusing on the functions that need to be fulfilled, rather than only the chemical performing them, it becomes possible to identify a broader range of functional alternatives, which in turn increases the likelihood of avoiding regrettable substitution.[18]

Many alternatives assessment frameworks were published to guide the evaluation, comparison and selection of suitable alternatives, but more research is still needed to ensure their proper implementation in concrete cases, especially when comparing alternatives which are not other chemical substances.[7,19] Among others, Bechu *et al.* (2024) argued that further work is also needed to "Advance and incorporate flexible and practical approaches for trade-off considerations in decision-making given the information available".[19] Additional work is needed to develop and implement a method which can support the assessor in their decision-making when comparing alternatives based on various aspects (*e.g.* technical performance, costs, environmental impacts). Many alternatives assessment frameworks suggest using multi-criteria decision analysis (MCDA) methods to face this challenge.[5,7,17] MCDA methods were developed to formalize common-sense reasoning for decision problems that are too complex to be addressed intuitively.[20,21] To date, several studies have applied MCDA methods in the context of an alternatives assessment to evaluate and compare chemical alternatives, but only based on their hazard profiles.[22–24] One additional study implemented MCDA methods to evaluate and compare chemical alternatives to lead used in solder based on a wider range of criteria, *i.e.* hazard profile, other environmental impacts (*e.g.* energy use; non-renewable material use *etc.*), physical hazard, technical feasibility, and economical feasibility.[25] On the other hand, LCA studies typically consider "functional equivalence" between alternatives, without the multiple technical performance criteria considered here.

The main purpose of this study is to adapt MCDA methods previously used in the context of alternatives assessment to allow comparison of functional alternatives to a chemical of concern based on their environmental impacts and their technical performance. The main objective is for the method to be as transparent as possible so the decision-maker would be able to be explicit about their preferences when evaluating the potential trade-offs that could arise between technical performance, and safety for human health and the environment. The specific case of fluorinated gases used as foam blowing agents in insulation materials will serve as a case study to illustrate the potential implementation of the developed method.

2. Method

The method of this study was inspired by the alternatives assessment framework from ECHA.[5] Fig. 1 presents an overview of the method followed. This section provides detailed information for each step.

2.1. Identification of the substances of interest and their functions

The method developed in this study was applied to those fluorinated gases which are defined as PFAS. For the purpose of the study, PFAS are defined as substances containing a fully fluorinated methyl ($-CF_3$) or methylene ($-CF_2-$) group in their molecular structure, as proposed by the Organisation for Economic Co-operation and Development (OECD)[26] and by the REACH restriction on uses of PFAS,[27] without their exclusion criteria. The purpose of this study is not to discuss whether all fluorinated gases covered by this definition represent similar concerns for human health and the environment. The substances used as fluorinated gases were identified based on the information available in the database of alternatives to PMT and PFAS developed as part of the European project ZeroPM.[28] The database was also used to determine the specific uses of fluorinated gases and the functions they deliver in each use. As the database was built around the functional substitution approach, it was also possible to determine the chemical

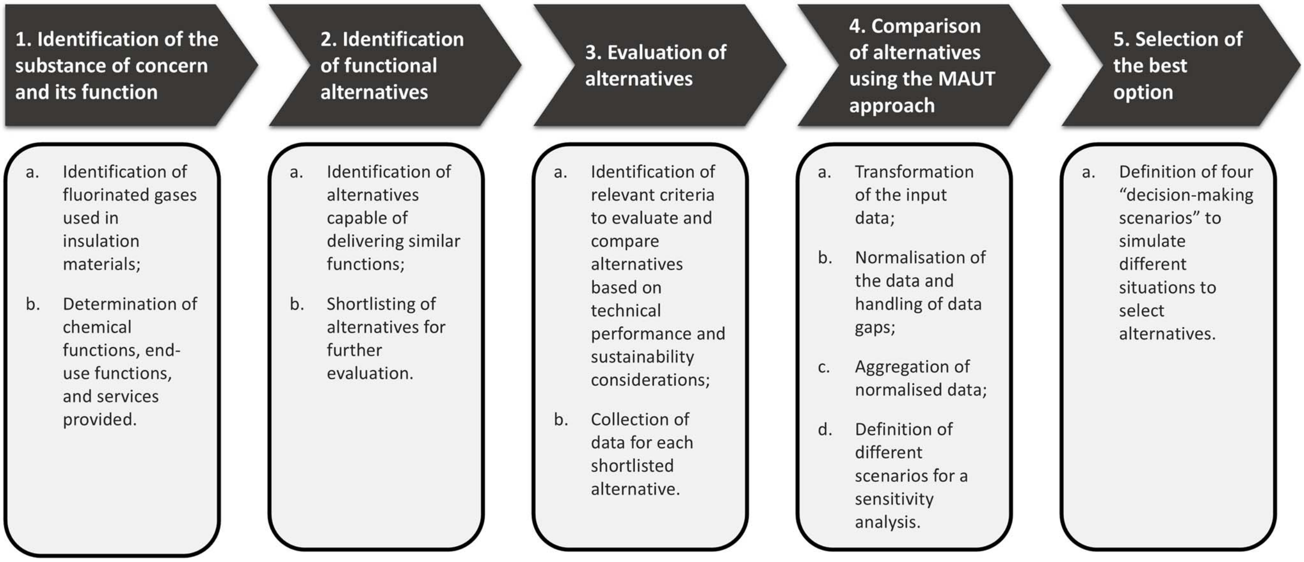

Fig. 1 Overview of the method followed in the study.

functions, end-use functions and services delivered by fluorinated gases for each use. For the purpose of this study, only the use of fluorinated gases as foam blowing agents was considered.

In order to be able to identify, evaluate and compare functional alternatives, a functional unit was defined based on the information collected on the uses and functions of fluorinated gases, following the approach commonly used in life cycle assessment (LCA). In the context of this study, a functional unit is defined as the amount of the substance of concern necessary in a specific product or process in order to deliver its primary function. Based on the information collected on the services delivered by PFAS as foam blowing agents, it can be concluded that a suitable alternative should be capable of providing a satisfactory thermal insulation for residential building applications (*e.g.* in a wall). The thermal properties of a wall are generally evaluated based on its thermal transmittance U (expressed in W m^{-2} K^{-1}), which is defined as the heat flow that passes through a unit area of a complex component due to a temperature gradient.[29] A functional unit was then defined as 1 m^2 of wall insulation with a thermal resistance of 1 m^2 K W^{-1}, which is the value generally taken to evaluate insulation materials.[30] Based on the functional unit, the total reference flow for each material is calculated, and from this, the cradle-to-gate LCA impacts are determined for comparative analysis.

2.2. Identification of potential functional alternatives

Potential functional alternatives to fluorinated gases were identified based on the information available in the ZeroPM database.[28] As insulation materials have been of particular interest to reduce the energy consumption of buildings, literature reviews of studies evaluating different insulation materials have already been published.[29,30] Those reviews served to complete the initial list of potential alternatives available in the ZeroPM database. Since the main goal of this study was to adapt these methods for evaluating alternatives that are not chemical substances, only non-chemical alternatives were considered for further assessment.

2.3. Evaluation of the identified alternatives

2.3.1. Identification of criteria to evaluate the alternatives. For this study, the identified alternatives were evaluated and compared based on their technical performance, and their environmental impacts along their life cycle. Economic feasibility of the identified alternatives was considered out of the scope as it is highly dependent on the stakeholder performing the alternatives assessment and cannot be generalized.

The specific criteria to evaluate the safety of the identified alternatives were selected by following the guidance of the OECD.[17] For this study, the term "safety" refers to endpoints related to their environmental impacts (*e.g.* global warming potential, ozone layer depletion potential). Specific criteria for the evaluation of the technical performance of the alternatives were determined based on the information collected in a previous study.[29] Given the high number of criteria identified for evaluation, criteria were gathered in different categories for each attribute, as explained in the SI (SI 1; Fig. SI 1.2).

2.3.2. Collection of data. Data collection strategies varied depending on the category of criteria, as described below. For each alternative and criterion, a single value was selected to construct the performance matrix. When multiple values were available for the same criterion and alternative, their average was used as the baseline scenario.

Technical performance attributes. As all identified alternatives are insulation materials already in use and available on the market,[29] it was considered that their adoption was feasible. In other words, all alternatives were considered technically feasible. The alternatives were then evaluated and compared only based on their capacity to deliver the required performance.

Data on the technical performance of the identified alternatives were collected based on the information collected in a review of studies evaluating the insulation performance of different insulation materials.[29]

Environmental impacts attributes. Data related to environmental impacts of the identified alternatives were collected based on LCA results on different insulation materials. There is a substantial body of literature on LCA applications for insulation materials already available,[30] and characterised (LCIA) results available in the Ecoinvent database Ecoinvent 3.9 with a cut-off methodology,[31] therefore no new assessment was performed for the purpose of this study.

The Ecoinvent database is a source of cradle-to-gate life cycle inventory data for about 20 000 products and processes. It means that the assessment focuses only on the potential environmental impacts of producing the insulating material, including all production-related emissions and waste. Therefore, waste generated during the material's use phase is not included, even though different materials might produce varying amounts of waste in real-life applications.

The geographical scope of the impact assessment is both global and European. This data set includes market data and accounts for transportation impacts. One of the key assumptions in this study is that the insulation materials under evaluation are equivalent in fulfilling the technical performance requirements over their design life without needing replacement. While different materials may have different lifespans, this study does not consider scenarios where a material might need replacement if it fails before the end of the application design life.

The study also does not factor in end-of-life impacts. The disposal processes for insulation materials such as landfilling, recycling, incineration, and incineration with energy recovery could depend on the kind of insulation material. Materials requiring disposal in hazardous waste landfills or incineration facilities due to the presence of toxic substances, like flame retardants, would likely have a higher end-of-life impact than those disposed of through conventional means. However, these aspects are beyond the scope of this study.

As a cut-off methodology was followed, any recycling processes are fed with raw materials (*i.e.* waste streams) free of any environmental burdens, and the product in focus does not get credits for the production of potential by-products.

The impacts are calculated using the Product Environmental Footprint (PEF) recommended life cycle impact assessment method EFv3.1 EN15804.[32] The IPCC 2021 method was also used as an impact indicator for the GWP of the materials.[33] In total, 14 different impact indicators were selected to compare the materials.

2.4. Comparison of the potential alternatives following multi-criteria decision analysis methods

2.4.1. Justification for using MAUT approach. Previous studies which implemented MCDA methods in the context of an alternatives assessment used the heat mapping, multi-attribute utility theory (MAUT), and ELECTRE III approaches.[22–25] Background information on the different types of MCDAs methods is available in the SI (SI 1). For the purpose of the study, only the MAUT approach was applied as previous studies demonstrated that it is easy to implement while still being transparent enough for the decision-maker to understand the basis for the final ranking of the alternatives.[34] In short, MAUT is an optimization approach which assumes that the decision-maker has an explicit and well-defined set of preferences, and that they are rationale and consistent in their preferences. This approach also assumes that the preferences are stable and transitive, which means that, if alternative A is better than alternative B, and alternative B is better than alternative C, then alternative A is better than alternative C.[25] More information on the theory of the MAUT method is available in the SI (SI 1).

2.4.2. Transformation of the data, normalisation, and handling of data gaps. In the MAUT method, a utility function is used to transform the collected data in the performance matrix into a dimensionless utility scale ranging from 0 to 1 in order to be able to compare them. In this normalised scale, 0 represents the worst outcome for a given criterion while 1 represents the best possible outcome. For each criterion, the worst performing alternative was assigned a score of 0, and the alternative which performs the best was assigned a score of 1. Performance data that lay between these extremes was normalised using a linear utility function, as in previous studies.[22–25] To ensure that the normalised data of the different alternatives are well distributed between 0 and 1 for one criterion, the collected quantitative data were log-transformed before the normalisation. More information about this step is available in the SI (SI 6).

In case of data gaps, a "risk neutral" approach was taken and a value of 0.5 was assigned in the normalised data, as suggested in previous studies.[22,24]

2.4.3. Aggregation of normalised data and ranking. As a baseline scenario, normalised data were aggregated by calculating the average score of each alternative across all the criteria, by assuming that each criterion has an equal weight in the decision. The alternatives were ranked based on this final score.

2.4.4. Sensitivity analysis. An analysis of the sensitivity of the final results based on the assumptions made on the input data and the handling of data gaps was performed. To that end, three different scenarios were defined as described below.

- "Neutral" approach: if several data points for one alternative in one criterion were available, the arithmetic average of the data was taken as the input; data gaps were assigned a score of 0.5 in the normalised data.

- "Optimistic" approach: if several data points for one alternative in one criterion were available, the data point representing the best case was selected as the input; data gaps were assigned a score of 0.8 in the normalised data.

- "Pessimistic" approach: if several data points for one alternative in one criterion were available, the data point representing the worst case was selected as the input; data gaps were assigned a score of 0.2 in the normalised data.

2.5. Decision-making scenarios

One of the main issues with the MAUT approach is that it allows for compensation between the different criteria in the aggregation step. In other words, a bad performance of an alternative in one criterion could be compensated by a good performance in another.[20,35] This may pose an issue in the context of an alternative assessment, as alternatives having a strong impact on the environment could still be ranked high if their technical performance is very good. Three different scenarios with different aggregation methods were tested and compared with the baseline scenario to investigate the influence of allowing compensation on the final ranking of alternatives:

- Baseline scenario: under the baseline scenario, both attributes (*i.e.* technical performance and environmental impacts) are considered simultaneously. Compensation between all criteria and between the attributes are allowed.

- No compensation scenario: under the no compensation scenario, both attributes are considered simultaneously. However, compensation is allowed only between criteria belonging in the same category (Table 1). No compensations between criteria categories and between the attributes are allowed, as proposed in a previous study.[34]

- Sequential scenario with technical performance considered first: in the first sequential scenario, the alternatives are first ranked based on the criteria belonging to the technical performance attribute. The five best alternatives are then evaluated based on the environmental impacts attribute, the others are eliminated from consideration, as proposed in a previous study.[25] No compensations between criteria categories are allowed.

- Sequential scenario with environmental impacts considered first: in the second sequential scenario, the alternatives are first ranked based on the criteria belonging to the environmental impacts attribute. The five best alternatives are then evaluated based on the technical performance attribute, the others are eliminated from consideration, as proposed in a previous study.[25] No compensations between criteria categories are allowed.

Table 1 summarizes how the scores for the different criteria categories and attributes, and the final scores were calculated for each decision-making scenario being tested, along the equations that were used for the calculations.

Table 1 Definition of different decision-making scenarios to compare functional alternatives[a]

Scenario	Score of criteria categories	Score of attributes	Final score
Baseline scenario	Arithmetic average of the scores from each criterion in the category n,i	Arithmetic average of the scores from each criteria category belonging to the attribute n	Arithmetic average of the scores from each attribute
	$x_{n,i} = \sum_{j=1}^{J_{n,i}} \frac{x_{n,i,j}}{J_{n,i}}$	$x_n = \sum_{i=1}^{I_n} \frac{x_{n,i}}{I_n}$	$X = \sum_{n=1}^{N} \frac{x_n}{N}$
Scenario without compensation	Arithmetic average of the scores from each criterion in the category n,i	Minimum score among all the criteria categories belonging to the attribute n	Minimum score among the scores of the attributes considered (here technical performance and environmental impacts)
	$x_{n,i} = \sum_{j=1}^{J_{n,i}} \frac{x_{n,i,j}}{J_{n,i}}$	$x_n = \min_{i=[1;\ I_n]} x_{n,i}$	$X = \min_{n=[1;\ N]} x_n$
Sequential scenario – technical performance attribute considered first	Arithmetic average of the scores from each criterion in the category n,i	Minimum score among all the criteria categories belonging to the technical performance attribute	For the 5 best alternatives on technical performance attribute: minimum score among all the criteria categories belonging to the environmental impacts attribute
	$x_{n,i} = \sum_{j=1}^{J_{n,i}} \frac{x_{n,i,j}}{J_{n,i}}$	$x_{\text{Tech}} = \min_{i=[1;\ I_{\text{Tech}}]} x_{\text{Tech},i}$	$X = \min_{i=[1;\ I_{\text{Env.}}]} x_{\text{Env.},i}$
Sequential scenario – environmental impacts attribute considered first	Arithmetic average of the scores from each criterion in the category n,i	Minimum score among all the criteria categories belonging to the environmental impacts attribute	For the 5 best alternatives on environmental impacts attribute: minimum score among all the criteria categories belonging to the technical performance attribute
	$x_{n,i} = \sum_{j=1}^{J_{n,i}} \frac{x_{n,i,j}}{J_{n,i}}$	$x_{\text{Env.}} = \min_{i=[1;\ I_{\text{Env.}}]} x_{\text{Env.},i}$	$X = \min_{i=[1;\ I_{\text{Tech}}]} x_{\text{Tech},i}$

[a] N is the total number of attributes, I_n the total number of criteria categories in the attribute n, and $J_{n,i}$ the total number of criteria in the criteria category i in the attribute; $x_{n,i,j}$ represents the score of the alternative being evaluated for the criterion j in the category i in the attribute n; X represents the total score of the alternative being evaluated.

3. Results and discussion

3.1. Identification of substances used, and identification of functional alternatives

According to the information available in the ZeroPM database, fluorinated gases have 6 different sub-uses. Only the sub-use of fluorinated gases as foam blowing agents was considered for the purpose of this study, as it is the second largest use of fluorinated gases in terms of tonnages used,[36] and because a lot of work regarding alternatives to fluorinated gases used in refrigeration and heat pumps applications (the first largest use of fluorinated gases) has already been done.[37] 12 different PFAS used as foam blowing agents could be identified. Those PFAS are used in 8 different applications, namely: rigid polyurethane foam, rigid polyurethane board and panels, rigid polyurethane spray foam, rigid polyurethane pipe-in-pipe and block foam, polyurethane integral skin, rigid closed-cell polyurethane insulation foam, extruded polystyrene foam, and phenolic foam.[28]

In all the applications mentioned, PFAS are used as foamant (chemical function) to ensure a good expansion of the insulation foam (end-use function). However, they deliver different services, depending on the end-products they are used in: they can ensure a good thermal insulation for residential and commercial construction applications (rigid polyurethane board and panels, and extruded polystyrene foam); ensure thermal insulation for refrigerators, freezers, cold rooms (rigid polyurethane foam), or for consumer applications, such as cushions or mattresses (polyurethane integral skin); ensure thermal insulation for structures with difficult access, *e.g.* around windows and doors, or around pipes (rigid polyurethane spray foam); prevent pipes from freezing and cracking (rigid polyurethane pipe-in-pipe and block foam, and rigid closed-cell polyurethane insulation foam); or ensure thermal insulation for industrial heating and ventilation systems (phenolic foam).[28] As proper insulation of residential buildings is one of the principal objectives of the European Green Deal for the Green Transition,[38,39] only the specific cases of PFAS used in insulation materials for residential construction applications were considered for this study, *i.e.*, PFAS used in rigid polyurethane board and panels (PU), and extruded polystyrene foam (XPS). According to the ZeroPM database, eight different PFAS are used in such insulation materials.[28] These substances of concern are listed in the SI (Table SI 2).

In the ZeroPM database, 7 alternative blowing agents (*e.g. n*-pentane, cyclopentane, isobutane), 2 alternative insulation foams (water blown foam, and cementitious foams), and 7 alternative insulation materials (*e.g.* fibreglass, cellulose, hemp) are listed as potential suitable alternatives for this particular application.[28] As this study aims to propose a method to evaluate and compare alternatives other than alternative substances, only the alternative materials were considered for evaluation. The list of potential alternative insulation materials was completed based on the information available in a review on insulation materials previously published.[29] In total, 33 insulation materials were identified as potential alternatives and are listed in the SI (Table SI 2).

By defining the three levels of function of a substance of concern (*i.e.* chemical function, end-use function, and service) following the functional substitution approach, it is possible to identify different types of alternatives, and to go beyond considering only chemical alternatives for substitution.[18] In this study, focusing solely on the chemical function of fluorinated gases in insulation materials would restrict the analysis to alternative substances that can act as foam blowing agents. By considering the service level instead, alternative insulation materials that do not require foam blowing agents can also be identified as potentially viable alternatives. Chemical alternatives assessment methods based on hazard assessment may be simpler and easier to apply when only other substances with similar physico-chemical properties are considered. One can argue that such methods might miss important aspects which an LCA can identify, and the argument is even stronger when aspects other than toxicological hazards are the main issues for non-chemical alternatives with a significantly different life cycle.

In this study, only PU- and XPS-containing fluorinated foam blowing agents were evaluated and compared with other insulation materials. As it was not possible to identify which specific fluorinated foam blowing agent was used in PU- and XPS insulation foams from the information available in the review,[29] it was considered that the technical performance data collected represent the average of the different fluorinated gases. A similar approach was taken when evaluating the environmental impacts of PU foams. For XPS foams, datasets were available in Ecoinvent 3.9 for XPS blown with HFC-134a and with HFC-152a. Hence the environmental impacts of XPS foams were evaluated in the optimistic, pessimistic, and average approaches: by taking the minimum impact of the two foams, the maximum impact, or the mean of both impacts, respectively. Further work should investigate whether PU and XPS foams produced with non-fluorinated blowing agents (*e.g.* pentane, cyclopentane) would be better alternatives, based on LCA considerations. Previous work tried to propose a framework to adapt LCA methodologies to the specific case of PFAS, and applied it to compare outdoor garments with different durable water repellents (DWR).[40,41] Future work could aim to implement our framework in this particular use case of PFAS.

3.2. Evaluation of the functional alternatives

When characterizing an insulation material, four different criteria are considered: its thermal insulation; its water vapor resistance; its resistance to fire; and its acoustic insulation.[29] The thermal insulation performance of a material is express by its thermal conductivity (in W m^{-1} K^{-1}), and its thermal diffusivity, which is the ratio between the thermal conductivity and the product of the density and the specific heat capacity of the material.[29] Therefore, the thermal conductivity, the density, and the specific heat of the materials were considered to evaluate its thermal insulation. The water vapor resistance is characterised by the water vapor diffusion resistance factor,[29] which was used to evaluate the humidity insulation of the materials. The classification of the materials under the European Standard EN

Table 2 Selected criteria for the evaluation of the identified alternatives

	Criteria category	Criteria (unit)	Best case
Performance	Thermal insulation	Thermal conductivity (W m^{-1} K^{-1})	The lower the better
		Specific heat (kg kg^{-1} K^{-1})	The higher the better
		Density (kg m^{-3})	The higher the better
	Humidity insulation	Water vapor diffusion resistance factor (dimensionless)	The higher the better
	Resistance to fire	Fire classification	Classification A
Environmental impacts	Impact on climate	IPCC 2021 climate change global warming potential GWP100 (kg CO_2 Eq.)	The lower the better
		EN15804 climate change global warming potential GWP100 (kg CO_2 Eq.)	The lower the better
	Ozone layer depletion potential	EN15804 ozone depletion ozone depletion potential ODP (kg CFC 11 Eq.)	The lower the better
	Other environmental impacts	EN15804 acidification accumulated exceedance AE (mol H Eq.)	The lower the better
		EN15804 eutrophication freshwater fraction of nutrients reaching freshwater end compartment P (kg P Eq.)	The lower the better
		EN15804 eutrophication marine fraction of nutrients reaching marine end compartment N (kg N Eq.)	The lower the better
		EN15804 eutrophication terrestrial accumulated exceedance AE (mol N Eq.)	The lower the better
	Ecotoxicity	EN15804 ecotoxicity freshwater comparative toxic unit for ecosystems CTUe (CTUe)	The lower the better
	Human toxicity	EN15804 human toxicity carcinogenic comparative toxic unit for human CTUh (CTUh)	The lower the better
		EN15804 human toxicity non carcinogenic comparative toxic unit for human CTUh (CTUh)	The lower the better
	Resources used	EN15804 energy resources non renewable abiotic depletion potential ADP fossil fuels (MJ net calorific value)	The lower the better
		EN15804 water use user deprivation potential deprivation weighted water consumption (m^3 world eq. deprived)	The lower the better
		EN15804 land use soil quality index (dimensionless)	The lower the better
		EN15804 material resources metals minerals abiotic depletion potential ADP elements ultimate reserve (kg Sb Eq.)	The lower the better

13501-1 was used to evaluate their resistance to fire.[29] Acoustic insulating effects are not considered as primary criteria for the choice of an insulation material for a wall.[29] Therefore, acoustic insulation characteristics of the materials were not considered in the evaluation of their technical performance. All the criteria used for the evaluation of the technical performance of the identified alternatives are listed in Table 2, together with a description of what is considered as "the best case".

As illustrated in Table 2, environmental impacts were gathered in 6 different categories: contributions to climate change; ozone layer depletion potential; other environmental impacts; ecotoxicity; human toxicity; and resource use. Not all environmental impact indicators of the EN15804 were included for the evaluation of the alternatives. Indicators for climate change from biogenic, fossil fuels, and land use were not included in the evaluation as it was considered that they were not independent from the overall climate change indicator "climate change global warming potential". Similarly, indicators for ionizing radiation, photochemical oxidant, and particulate matter were not considered. A description of the "best case" for each criterion is provided in Table 2. All the information regarding the collection of the LCA data for the identified alternatives is provided in the SI (SI 3).

Only alternatives with data available for all criteria listed above were selected for further evaluation. The list of shortlisted alternatives being considered is available in the SI (Table SI 4.1). Recycled textile-based insulation materials were still included for evaluation despite the lack of data on their environmental impacts to evaluate the effect of data gaps on the outcome of the proposed method. All the technical performance data collected for the shortlisted alternatives are available in the SI (Table SI 4.2). The characterization factors for each shortlisted alternative and for all impact categories listed in Table 2 are provided in the SI (Table SI 4.3). The life cycle impacts were determined by calculating the total amount of material needed to fulfil the functional unit. More information about these calculations are provided in the SI (SI 4). The life cycle impacts for each shortlisted alternative and for all impact categories following the neutral, optimistic, and pessimistic approaches are provided in the SI (Table SI 4.4).

Previous studies already investigated how MCDA approaches could be used to evaluate and compare chemical alternatives[22–25] which is why the present study only focuses on non-chemical alternatives here. The safety of the chemical alternatives was evaluated based on their toxicological profile and their degradation in the environment by using QSAR-based predictions and experimental data on various human health and freshwater organisms toxicological endpoints.[22–24] Such an approach can become complicated when considering complex materials. To properly evaluate the material's safety, the assessor would need information on the identity and toxicological profiles of all constituents, as well as potential mixture effects, which can introduce substantial uncertainty into the assessment. In comparison, we believe that the uncertainty related to the potential hazard on human health and freshwater organism is lower by using an LCA as the life cycle impact assessments characterisation factors for human health and ecotoxicity are based on mammalian rodent experimental data and freshwater experimental organism data (respectively) instead of QSAR predictions. Additionally, LCA allows to consider potential changes in exposure in the assessment by evaluating impacts of alternatives for diverse environmental impact categories, therefore preventing a potential shift of burden on the environment. Furthermore, by calculating characterization factors per functional unit, LCA allows to consider differences in performance among the alternatives when evaluating their impacts on the environment, which would not be possible if the alternatives were evaluated only based on a hazard assessment. Although not perfect due to the uncertainty in the results, we felt that comparing the environmental impacts of the materials based on LCA results was more appropriate in the context of this study.

Numerous LCA studies on insulation materials have already been performed,[30] which facilitated the collection of data for the evaluation of the different alternatives. This suggests that safety evaluation methods in an alternatives assessment can be adapted to the type of alternative being considered, and that obtaining data for all endpoints listed in the OECD guidance may not always be necessary.[17] The MAUT approach proposed here can easily be adapted to consider different types of criteria (*i.e.* LCA results or toxicological profiles) depending on the type of alternatives that is being evaluated.

In the present study, a "min–max" approach was followed by defining a "best case" and "worst case" for each criterion under consideration based on the best performing (respectively, least performing) alternative in each criterion.[42] These were used for the normalisation of the data into a dimensionless scale ranging from 0 to 1 by assigning a score of 1 (respectively, 0) to the best (respectively, worst) case. This method is also referred to as "internalised normalisation" in a previous study.[25] Although this approach is well suited for properly differentiating alternatives and clearly identify candidates which are performing better for a given criterion, it can also over-penalize an alternative even though it does not present any concern in regards to the specific criterion being considered. For instance, for the human non-carcinogenic toxicity impact category of the LCA, sheep wool got assign the score of 0 in the baseline scenario because it has the highest impact compared to the other alternatives, even though it is in the range of 10^{-7} CTUh which tends to indicate that sheep wool does not present a high concern in regards to human toxicity. This issue could be avoided by determining the "best" and "worst" cases based on standard threshold values that are independent from the set of values of the alternatives. By doing so, the alternative performing worst for a given criterion could still have a good score for that criterion which might influence its final ranking. This could be particularly relevant for sheep wool which is the worst performing alternative for several environmental impact categories, hence scoring 0 in several criteria. Such an approach was taken in the previous studies focusing on chemical alternatives by using the threshold values from the Green Screen method and from the REACH Regulation to set the "worst" cases for the toxicological endpoints.[22,24] Further work should investigate

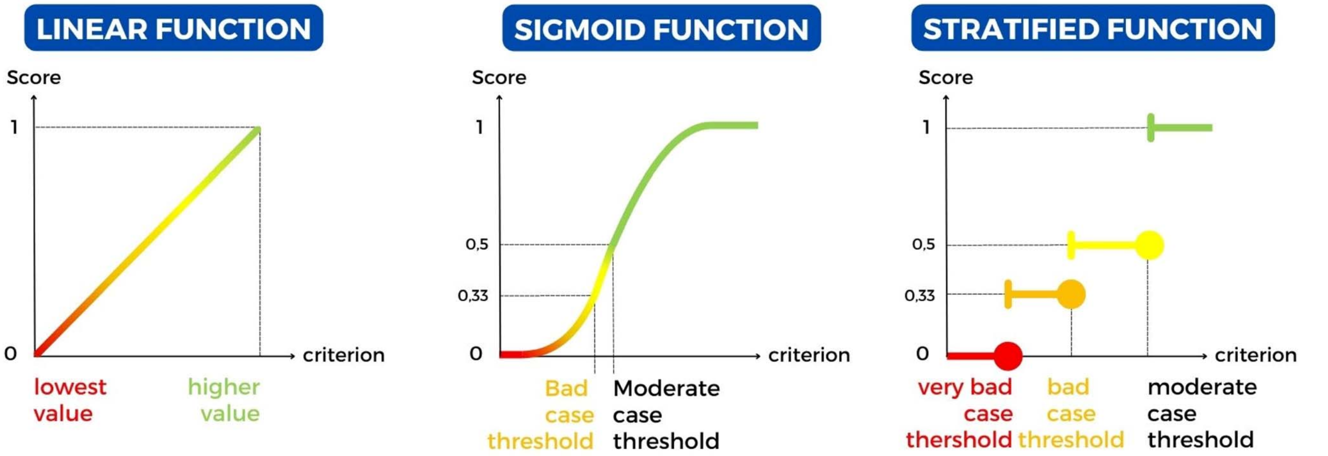

Fig. 2 Potential utility functions to better capture the preferences of a decision-maker.

whether such thresholds could be determined for the different impact categories included in an LCA.

Furthermore, in this study only a linear utility function was used to normalise the data. A linear function presents the advantage of being easy to use, but it does not provide much information on the preferences of the assessor. It could be changed to better capture situations where the decision-maker is not concerned about the performance of an alternative for a specific criterion as long as it is above or below a certain threshold value.[25] For instance, in the baseline scenario, hemp-based material was assigned a score of 0 for its thermal conductivity as it is the highest among the alternatives considered. However, it is possible that in some situations, a thermal conductivity of 0.049 W m^{-1} K^{-1} is satisfactory, which would mean that hemp-based material could still be considered as a potential viable alternative. If that is the case, hemp-based material should get a normalised score close to 1, even if it is the worst performing alternative. To prevent this issue, the decision-maker could use a stratified, or a sigmoidal utility function instead (Fig. 2). By doing so, an alternative which is not performing well in one criterion, but is still "good enough" in regards to the requirements of the decision-maker will not be over-penalized. To do so, the assessor must determine threshold values for each criterion to classify the alternatives as very bad, bad, satisfactory, or "best-in-class". This approach is particularly relevant in regards to the evaluation of the technical performance of the alternatives to avoid eliminating a candidate for consideration because its performance is not "best-in-class", even though it might still perform well enough for the specific conditions of use. However, such an approach requires knowledge of what can be considered as "acceptable" for the different criteria being considered. In other research areas, previously developed 'satisficing' decision-making models aim to achieve satisfactory performance on each criterion while taking into account the criteria's relative importance[43,44] This paradigm could be adapted and applied to the specific context of alternatives assessment. As suggested in a previous study, regulatory bodies could define minimum requirements that alternatives must meet to be considered 'acceptable' in terms of performance.[45] In some use cases, industrial standards are established for materials to provide additional guidance and ensure compliance.

3.3. Comparison of alternatives

Table 3 provides an overview of the final ranking of the different short-listed alternatives following the different decision-making scenarios which were defined. All data which was used and each MAUT model used to obtain those rankings are available in the SI (Tables SI 5, 6.1, 6.2, 7, 8 and 9).

3.3.1. Baseline scenarios. Under the baseline scenarios, all criteria were considered simultaneously with an equal weight for the final decision. As shown in the SI (Tables SI 6.1 and 6.2), no alternatives perform well across all properties under consideration. For instance, under the neutral scenario, XPS and PU are the best regarding the insulation performance, but they respectively rank 10 and 9 with regard to their environmental impacts. Conversely, EPS and cellulose-based insulation materials rank best based on their environmental impacts, but they are respectively ranked 5 and 7 in regard to their insulation performance. Under the neutral approach, EPS, cellulose-based material, and fibreglass emerge as the preferred alternatives when considering all the criteria related to environmental impacts and insulation performance.

The effect of the selection of the input data on the final ranking can be evaluated by comparing the neutral, optimistic and pessimistic approaches. The differences in the final ranking of PU, XPS, EPS, cellulose, cork and sheep wool according to these approaches was lower than 2, which indicates that the evaluation of those alternatives was not highly influenced by the choice of the data input. On the other hand, fibreglass is ranked 3rd under the neutral approach, 6th under the optimistic approach, and 2nd under the pessimistic approach, which could influence the final conclusion as fibreglass would be considered as a "safer alternative" under the neutral and pessimistic approaches, but not under the optimistic approach, emphasizing the importance of considering the uncertainty in the input data when evaluating alternatives following the MAUT method. This becomes even more

Table 3 Final ranking of the functional alternatives to fluorinated gases used in insulation materials following the different decision-making scenarios[a]

	Baseline scenario			No compensation and no trade-off			Alternatives with good performance are preferred			Alternatives with low environmental impacts are preferred		
	N	O	P	N	O	P	N	O	P	N	O	P
XPS	**5**	**3**	**5**	**10**	**2**	**8**	**4**	**NA**	**4**	**NA**	**2**	**NA**
PU	**6**	**8**	**8**	**6**	**10**	**4**	**NA**	**4**	**4**	**NA**	**NA**	**NA**
EPS	1	2	1	3	6	3	NA	NA	1	5	4	4
Fibreglass	3	6	2	1	4	1	2	2	2	2	NA	2
Rock wool	4	7	3	4	7	2	3	4	3	1	NA	1
Cellulose	2	1	4	2	1	7	1	1	NA	4	1	3
Hemp	8	5	6	9	9	8	NA	NA	NA	NA	NA	NA
Cork	7	9	9	5	3	6	4	3	NA	NA	NA	NA
Wood fibres	9	10	7	8	5	8	NA	NA	NA	NA	5	4
Sheep wool	11	11	11	10	10	8	NA	NA	NA	NA	NA	NA
Recycled textile	10	4	10	7	8	5	NA	NA	NA	4	3	NA

[a] NA: alternative not assessed because it was not among the top 5 candidate after the first sequence of the assessment, N: neutral; O: optimistic; P: pessimistic.

important for alternatives with many gaps in the input data as shown by the example of recycled textile which is ranked 10th in the neutral and pessimistic approaches, but 4th in the optimistic approach. Future work should focus on incorporating a quantified evaluation of input data uncertainty into the MCDA model.

3.3.2. "No compensation" scenarios. The "no compensation" scenarios were defined to prevent potential concerns regarding the evaluated alternatives being hidden when calculating the final score. Under the neutral approach, it appears that some alternatives like EPS, and hemp-based materials are ranked worse compared to the baseline scenario. The difference in ranking for cellulose-based material is even more pronounced under the pessimistic approach, as it is ranked 4th under the baseline scenario while it is ranked 7th when not allowing for compensation. By having a closer look at the data in the SI (Table SI 7), it appears that cellulose-based materials do not perform well with regard to humidity insulation.

On the other hand, some alternatives such as fibreglass are ranked better under the scenario which does not allow for compensation compared to the baseline. Fibreglass is ranked 1st under the former scenario. This indicates that even though it is not perfect, it most likely does not present major concerns, and could be considered as the best compromise when considering all the criteria.

3.3.3. Sequential evaluation scenarios. Under the previous scenarios, alternatives performing badly in one of the criteria being evaluated were still considered in the final ranking. In other words, no criteria were used as threshold factors to eliminate alternatives. As done in a previous study, sequential scenarios were defined to test the effect of considering performance and environmental impacts as threshold factors on the final ranking of the alternatives.[25]

By considering the technical performance as a threshold factor (Table SI 8), the cellulose-based materials, fibreglass, and rock wool are ranked respectively, 1, 2, and 3. On the other hand, cork-based materials and XPS were ranked higher compared to the baseline scenario, indicating that they present a better technical performance, but their environmental impacts are also probably higher than the other alternatives being evaluated. If the environmental impacts are used as a threshold factor (Table SI 9), both cork-based materials, and XPS are eliminated from consideration which confirms this hypothesis. Under the neutral scenario, cellulose-based materials, rock wool, and fibreglass are the only alternatives which are not eliminated for consideration when either technical performance or environmental impacts are considered as threshold factors, which indicates that they are satisfactory from both perspectives.

3.3.4. Identification of suitable alternatives to insulation materials containing fluorinated gases. Based on the final ranking presented in Table 3, alternatives that are rank better than XPS and PU can be identified in every possible scenario, which indicates that suitable alternatives to fluorinated gases used in insulation materials are available. On the other hand, sheep wool is consistently ranked worse than both XPS and PU in every scenario, which suggests that it is a potential regrettable substitute. It is important to note that the environmental impacts of the different alternatives were evaluated without taking into considerations the impacts during the use phase and the end of life of the insulation materials. Such considerations may influence the final ranking of the alternatives and should be the focus of further work.

3.3.5. Preferences of the decision-maker through the aggregation method. In the present study, different aggregation methods were tested to simulate different decision-making scenarios. Those aggregation methods can be adapted to specify the preferences of the assessor in regards to the criteria being considered in the evaluation. In the present study, it was considered that every criterion being considered was of equal importance for the final decision by assigning a weight of 1 for every criterion to calculate the final score. Further work should investigate how the weighing of the different criteria would influence the final ranking of the different alternatives when considered simultaneously.

In this study, two different sequential approaches were tested to evaluate whether the final ranking of the alternatives would change if the technical performance and the environmental impacts would act as "threshold factors". Those scenarios represent fictional decision-making scenarios in which either the technical performance, or the environmental impacts of the alternatives are the highest priority for the assessor.

It is also possible to consider the criteria as "threshold factors" in a "simultaneous approach" by calculating the final score of an alternative using a geometric mean instead of an arithmetic mean. In that way, if an alternative score is 0 in one the criteria being considered, its final score will automatically be 0, and it will be eliminated for further consideration. However, such approach cannot be combined with an "internalised normalisation" as there is a probability that several alternatives will score 0 for at least one criterion just because they are the least performant compared to the other alternatives, which means that they would get a final score of 0. It would be difficult to properly rank all the alternatives if too many of them have the same final score. It is therefore preferable to use a geometric mean only in the case where the data is normalised based on external standard reference values, as explained previously.

3.4. MAUT provides a good framework to explicit relevant choices and preferences in alternatives assessment

MCDA approaches are promising methods to guide decision-making in an assessment of alternatives.[5,25] This study focused on the MAUT approach to investigate how its flexibility could be of use in practice for an alternative assessment, and how it allows to consider different perspective in such assessment. However, it emphasizes how choices that the decision-maker needs to take on the input data, the potential threshold values for the different criteria, the utility function, and the final aggregation method influence the final ranking of the alternatives, which may have a significant impact on concluding whether suitable safer alternatives to a substance of concern are available or not.

This might be highly relevant in a regulatory context as the availability of suitable alternatives is a critical part in the decision-making on bans of harmful substances. It is therefore important that such choices are made as explicit and transparent as possible so it is possible for a third party to understand what the preferences of the assessor are in order to properly understand why an alternative could be considered as viable or not. Such a tool could be helpful to ensure that results from alternatives assessment are properly considered in regulatory decisions. Furthermore, the proposed approach could be used to identify the environmental impacts hotspots of the different alternatives by using the LCA data to inform the decision makers where potential environmental may lead to when implementing an alternative. Such investigation should be the focus of further research.

4. Conclusions

The study aimed at adapting the MAUT method to evaluate and compare non-chemical alternatives to fluorinated gases used as foam blowing agents in insulation materials. By assessing both insulation performance and environmental impacts across the life cycle, the results indicate that viable alternatives to PFAS-based blowing agents are available. Furthermore, the study demonstrates how the MAUT approach can be employed to systematically incorporate decision-makers' requirements and preferences when assessing alternatives to substances of concern. Such an approach is highly relevant in regulatory context to ensure that results from alternatives assessments are properly considered in the decision-making process.

Author contributions

RF designed study, collected and analysed the data, and wrote the manuscript the manuscript with contributions from all the co-authors. OK and RA contributed to the collection of the data. All authors contributed to the discussions, reviewed and approved the final manuscript.

Conflicts of interest

The authors declare that they have no competing interests.

Data availability

The extracted data supporting the analysis and conclusions of this paper is included as part of the supplementary information (SI). Supplementary information: the method used for the analysis and on the collection of LCA data. See DOI: https://doi.org/10.1039/d5su00751h.

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