

# Do we need to use hazardous chemicals in society?

The implementation of the "Essential-Use" Concept

Romain Figuière





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Academic dissertation for the Degree of Doctor of Philosophy in Environmental Sciences at Stockholm University to be publicly defended on Friday 7 March 2025 at 13.00 in DeGeersalen, Geovetenskapen hus Y, Svante Arrhenius väg 14, and online via Zoom, public link is available at the department website.

### Abstract

Chemical legislation serves as an important regulatory tool to protect human health and the environment from the risks posed by substances of concern. Discussions at the EU level have focused on implementing the “essential-use” concept in chemical regulations to improve their efficiency. In short, a use of a substance of concern should be permitted only if it is deemed “essential” – that is, if it is necessary for health, safety, or critical for the functioning of society, and that there is no safer alternative available. Although the European Commission recently published guiding criteria to consider for implementing the “essential-use” concept as a tool to guide decision-making, more work is needed to investigate its practical implementation.

By taking the examples of uses of per- and polyfluoroalkyl substances (PFAS) (**Paper I and III**), three persistent, mobile, and toxic (PMT) substances (i.e. allura red, benzophenone-4, and climbazole) (**Paper II**), and microplastics (**Paper IV**), this thesis aims to determine the type and amount of information needed to make a proper essentiality assessment. The functional substitution approach was followed to determine the chemical functions provided by the case study substances in their respective uses, and how these functions are linked with the services the substances provide in the end product. Based on this information, one use of allura red (**Paper II**), and two uses of microplastics (**Paper IV**) were deemed “non-essential” as the functions delivered by the substances are not necessary for the technical performance of the end product. Existing alternatives assessment frameworks were followed to identify, evaluate, and compare potential alternatives to the substances of interest to determine if suitable alternatives were available for the uses being considered. Suitable and safer alternatives could be identified for 28 uses of PFAS (**Paper I and III**), for all uses of allura red, benzophenone-4, and climbazole (**Paper II**), and for seven uses of microplastics (**Paper IV**), which were deemed “non-essential”.

This thesis also evaluates how the “essential-use” concept differs from current chemical legislation, and the implications of implementing such a concept to guide decision-making by taking the examples of the Stockholm Convention and the REACH Regulation. The analysis suggests that no fundamental changes are needed in regulatory requirements to implement the “essential-use” concept as authorities already have the capacity to gather the relevant information needed to determine if a use is (non-)essential. However, good cooperation with industry throughout the value chain is necessary for the competent authorities to properly understand the true purpose a substance of concern serves in the end product (**Paper IV**). Overall, the results suggest that the “essential-use” concept can be a valuable tool which presents the potential to speed-up the decision-making by focusing on identifying the non-essential uses of substances of concern.

**Keywords:** *Chemical risk management, Functional substitution approach, Alternatives assessment, Multicriteria decision analysis, REACH Regulation.*

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"The best way to change what we do is to change how we think."

- Paul Anastas



# Abstract

Chemical legislation serves as an important regulatory tool to protect human health and the environment from the risks posed by substances of concern. Discussions at the EU level have focused on implementing the “essential-use” concept in chemical regulations to improve their efficiency. In short, a use of a substance of concern should be permitted only if it is deemed “essential” – that is, if it is necessary for health, safety, or critical for the functioning of society, and that there is no safer alternative available. Although the European Commission recently published guiding criteria to consider for implementing the “essential-use” concept as a tool to guide decision-making, more work is needed to investigate its practical implementation.

By taking the examples of uses of per- and polyfluoroalkyl substances (PFAS) (**Paper I and III**), three persistent, mobile, and toxic (PMT) substances (i.e. allura red, benzophenone-4, and climabazole) (**Paper II**), and microplastics (**Paper IV**), this thesis aims to determine the type and amount of information needed to make a proper essentiality assessment. The functional substitution approach was followed to determine the chemical functions provided by the case study substances in their respective uses, and how these functions are linked with the services the substances provide in the end product. Based on this information, one use of allura red (**Paper II**), and two uses of microplastics (**Paper IV**) were deemed “non-essential” as the functions delivered by the substances are not necessary for the technical performance of the end product. Existing alternatives assessment frameworks were followed to identify, evaluate, and compare potential alternatives to the substances of interest to determine if suitable alternatives were available for the uses being considered. Suitable and safer alternatives could be identified for 28 uses of PFAS (**Paper I and III**), for all uses of allura red, benzophenone-4, and climabazole (**Paper II**), and for seven uses of microplastics (**Paper IV**), which were deemed “non-essential”.

This thesis also evaluates how the “essential-use” concept differs from current chemical legislation, and the implications of implementing such a concept to guide decision-making by taking the examples of the Stockholm Convention and the REACH Regulation. The analysis suggests that no fundamental changes are needed in regulatory requirements to implement the “essential-use” concept as authorities already have the capacity to gather the relevant information needed to determine if a use is (non-)essential. However, good cooperation with industry throughout the value chain is necessary for the competent authorities to properly understand the true purpose a substance of concern serves in the end product (**Paper IV**). Overall, the results suggest that the “essential-use” concept can be a valuable tool which presents the potential to speed-up the decision-making by focusing on identifying the non-essential uses of substances of concern.

# Sammanfattning

Lagstiftning är ett viktigt verktyg för att skydda människors hälsa och miljön från riskerna med farliga kemikalier. Diskussioner inom EU har kretsat kring hur man kan tillämpa konceptet ”Essential Use”, ”nödvändig användning” på svenska, i kemikalierereglering för att göra den mer effektiv. Enkelt uttryckt innebär Essential Use att farliga kemikalier endast ska användas om dess användning bedöms som ”essential” eller ”nödvändig” – det vill säga, om det är avgörande för hälsa, säkerhet eller samhällets funktion och om inga säkrare alternativ finns tillgängliga. EU-kommissionen har nyligen publicerat en vägledning som syftar till att främja implementering av konceptet i olika beslutsprocesser, men många frågor återstår innan konceptet fullt ut kan tillämpas i praktiken.

I den här avhandlingen analyseras praktiska exempel på användning av per- och polyfluoralkylsubstanser (PFAS) (**Paper I och III**), persistenta, mobila och toxiska substanser (PMT) (dvs. allurarött, bensofenon-4 och klimabazol) (**Paper II**), samt mikroplaster (**Paper IV**). Syftet är att undersöka vilken typ och mängd information som behövs för att göra en korrekt bedömning av en kemikalies ”nödvändighet”. Med hjälp av en metod för funktionell substitution analyserades vilka funktioner de undersökta kemikalierna hade i sina respektive användningsområden, och hur dessa funktioner var kopplade till den huvudfunktion som kemikalierna bidrog till i slutprodukten. Utifrån denna analys klassificerades en användning av allurarött (**Paper II**) och två användningar av mikroplaster (**Paper IV**) som ”icke-nödvändiga” eftersom de funktioner kemikalierna bidrog med inte var ”nödvändiga” för slutprodukten tekniska prestanda. Vidare användes befintliga metoder för bedömning av alternativ för att identifiera, utvärdera och jämföra potentiella ersättningsalternativ till de undersökta kemikalierna. Lämpliga och säkrare alternativ kunde identifieras för 28 användningar av PFAS (**Paper I och III**), för alla användningar av allurarött, bensofenon-4 och klimabazol (**Paper II**) och för sju användningar av mikroplaster (**Paper IV**). Alla dessa användningar bedömdes således som ”icke-nödvändiga”.

Avhandlingen granskar också hur implementering av Essential Use konceptet skulle förändra nuvarande kemikalielagstiftning. Med exempel från Stockholmskonventionen och REACH-förordningen jämfördes tidigare beslut om riskhantering med de potentiella beslut som skulle kunna uppstå om Essential Use konceptet tillämpats. Analysen visar att inga förändringar i nuvarande regulatoriska processer behövs för att implementera konceptet, eftersom myndigheter redan har möjlighet att samla in relevant information för att avgöra om en användning är ”nödvändig” eller ej. Däremot krävs ett samarbete med industrin genom hela värdekedjan för att myndigheterna ska få en djupare förståelse för kemikaliernas faktiska funktion i slutprodukten (**Paper IV**). Sammantaget visar resultaten att konceptet Essential Use kan vara ett användbart

verktyg som kan bidra till att effektivisera beslutsprocesser genom att identifiera "icke-nödvändiga" användningar av farliga kemikalier.

# Résumé

Les législations sur les produits chimiques sont des outils réglementaires essentiels pour protéger la santé humaine et l'environnement contre les risques posés par les substances chimiques préoccupantes. À l'échelle européenne, des discussions sont en cours pour mettre en œuvre le concept d'« usage essentiel » dans le but d'améliorer ces réglementations. En résumé, l'utilisation d'une substance préoccupante ne devrait être autorisée que si elle est jugée « essentielle », c'est-à-dire nécessaire pour la santé, la sécurité ou le fonctionnement de la société, et s'il n'existe aucune alternative plus sûre. Bien que la Commission européenne ait récemment publié des critères d'évaluation pouvant servir pour appliquer le concept d'« usage essentiel » comme un outil pour orienter les décisions, des travaux supplémentaires sont nécessaires pour examiner sa mise en œuvre en pratique.

En prenant des exemples d'usages des substances per- et polyfluoroalkyles (PFAS) (**Article I et III**), trois substances persistantes, mobiles et toxiques (PMT) (i.e. allura rouge, benzophenone-4, et climbazole) (**Article II**) et des microplastiques (**Article IV**), ce travail vise à déterminer le type et la quantité d'informations qui seraient nécessaires pour évaluer correctement l'essentialité d'un usage. Une approche basée sur la substitution fonctionnelle a été adoptée pour déterminer les fonctions chimiques fournies par les substances étudiées dans leurs utilisations respectives, ainsi que la manière dont ces fonctions sont liées aux services qu'elles rendent dans le produit final. Sur la base de ces informations, un usage d'allura rouge (**Article II**) et deux usages de microplastiques (**Article IV**) ont été jugés comme « non essentielles », car les fonctions qu'elles remplissent ne sont pas nécessaires pour que le produit final puisse délivrer ses services. Des méthodes déjà existantes pour l'évaluation des alternatives ont été suivies dans le but de pouvoir identifier, évaluer et comparer les alternatives potentielles aux substances concernées, afin de déterminer si des alternatives adaptées étaient disponibles pour les usages évalués. Des alternatives satisfaisantes et plus sûres ont été identifiées pour 28 usages de PFAS (**Article I et III**), pour tous les usages de allura rouge, benzophenone-4, et climbazole (**Article II**), et sept usages de microplastiques (**Article IV**), qui ont été jugés « non essentielles ». Cette thèse évalue également en quoi le concept d'« usage essentiel » diffère des réglementations chimiques actuelles et quelles seraient les implications de l'intégration de ce concept dans ces procédés réglementaires en prenant les exemples de la Convention de Stockholm et du règlement REACH. L'analyse suggère qu'aucun changement fondamental des processus réglementaires n'est nécessaire pour mettre en œuvre le concept d'« usage essentiel », car les autorités compétentes sont déjà en capacité de collecter les informations pertinentes nécessaires pour

déterminer si un usage est (non) essentielle. Cependant, une bonne coopération avec l'industrie tout au long de la chaîne de valeur de la substance d'intérêt est essentielle pour que les autorités compétentes comprennent réellement le rôle joué par cette substance dans le produit final.

En conclusion, les résultats suggèrent que le concept d'« usage essentiel » peut constituer un outil précieux, capable d'accélérer le processus de prise de décision en se concentrant sur l'identification des utilisations non essentielles des substances préoccupantes.

# List of papers

The following papers are included in the thesis and referred to in the text by their Roman numerals indicated below. In order to save space in this document, the supporting data of each paper is provided in separate Excel files.

I – **Figuière, R.**, Miaz, L., Savvidou, E., & Cousins, I. (2025). An Overview of Potential Alternatives for the Multiple Uses of Per-and Polyfluoroalkyl Substances. *Environmental Science and Technology*.

II – van Dijk, J., **Figuière, R.**, Dekker, S. C., van Wezel, A. P., & Cousins, I. T. (2023). Managing PMT/vPvM substances in consumer products through the concepts of essential-use and functional substitution: a case-study for cosmetics. *Environmental Science: Processes & Impacts*, 25(6), 1067-1081.

III – **Figuière, R.**, Kirik, O., Aggarwal, R., Peters, G., & Cousins, I. T.. Assessment of functional alternatives to fluorinated foam blowing agents in insulation materials. Manuscript format.

IV – **Figuière, R.**, Wang, Z., Glüge, J., Scheringer, M., Siegrist, A., & Cousins, I. T. Implications for Implementing the “Essential-Use” Concept in Chemical Legislation. Manuscript under review.

## List of papers mentioned but not included in the thesis

1. **Figuière, R.**, Borchert, F., Cousins, I. T., & Ågerstrand, M. (2023). The essential-use concept: a valuable tool to guide decision-making on applications for authorisation under REACH? *Environmental Sciences Europe*, 35(1), 5.
2. Borchert, F., **Figuière, R.**, Cousins, I. T., Rudén, C., & Ågerstrand, M. (2024). Identifying non-essential uses to phase out substances of very high concern under REACH. *Frontiers in Toxicology*, 6, 1488336.

# Author contribution to the papers

I – I designed the study, collected and analyzed the data. I wrote the manuscript with inputs from all co-authors.

II – I provided input to the development of the method. I collected and analyzed the data for one of the case study substances. I participated in the writing of the manuscript.

III – I designed the study, collected and analyzed the data. I wrote the manuscript with inputs from all co-authors.

IV – I participated in designing the study, as well as the collection and analysis of the data. I wrote the manuscript with inputs from all co-authors.

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# List of abbreviations

<b>AfA</b>	Application for Authorisation
<b>CFCs</b>	Chlorofluorocarbons
<b>CLP</b>	Classification, Labelling, and Packaging
<b>CMR</b>	Carcinogenic, mutagenic, or toxic to reproduction
<b>COP</b>	Conference of Parties
<b>CosIng</b>	Cosmetic Ingredients
<b>CSS</b>	Chemical Strategy for Sustainability
<b>ECHA</b>	European Chemicals Agency
<b>HFCs</b>	Hydrofluorocarbons
<b>HFOs</b>	Hydrofluoroolefins
<b>HFPO-DA</b>	Hexafluoropropylene oxide dimer acid
<b>IVD</b>	<i>In-vitro</i> diagnosis
<b>LCA</b>	Life cycle assessment
<b>MAUT</b>	Multi-attributes utility theory
<b>MCDA</b>	Multicriteria decision analysis
<b>OECD</b>	Organisation for Economic Co-operation and Development
<b>PBT</b>	Persistent, bioaccumulative, and toxic
<b>PMT</b>	Persistent, mobile, and toxic
<b>PFAS</b>	Per- and polyfluoroalkyl substances
<b>PFOA</b>	Perfluorooctanoic acid
<b>POPs</b>	Persistent organic pollutants
<b>POPRC</b>	POPs Review Committee
<b>PU</b>	Rigid polyurethane
<b>RAC</b>	Committee for Risk Assessment
<b>REACH</b>	Registration, Evaluation, Authorisation, and Restriction of Chemicals
<b>SEAC</b>	Committee for Socio-Economic Analysis
<b>SVHC</b>	Substances of very high concern
<b>TFA</b>	Trifluoroacetic acid
<b>vPvB</b>	Very persistent, and very bioaccumulative
<b>vPvM</b>	Very persistent, and very mobile
<b>XPS</b>	Extruded polystyrene

# 1. Introduction

## 1.1. The world of chemicals

Synthetic chemicals are used extensively in modern society, playing roles in consumer products, agriculture, pharmaceuticals, and various industrial and manufacturing processes. It was recently estimated that over 350 000 different chemicals and mixtures of chemicals are registered for production and use worldwide (Wang et al. 2020). While chemicals are used for their desired properties in products and processes, they may be released into the environment along their life cycle and cause harm to human health and ecosystems. Chemical pollution has been identified as one of the nine “planetary boundaries” (Rockström et al. 2009; Steffen et al. 2015), and it was recently estimated that this particular boundary has already been exceeded as the annual production and release of chemicals are increasing at a pace that outstrips the global capacity for assessment and monitoring (Persson et al. 2022). This highlights the need for implementing better measures to manage the potential risks posed by the vast number of chemicals on the global market.

## 1.2. Chemical risk management measures

Risk management measures are preventive methods that can be implemented to prevent exposure to hazardous chemicals and protect human health and ecosystems from adverse effects (KEMI 2020; Occupational Safety and Health Administration 2024). These measures can be classified into five categories (Occupational Safety and Health Administration 2024):

- *Personal Protective Equipment*: Requirement that people handling chemical substances wear protective equipment (e.g., gloves, lab coat) to prevent direct contact with substances of concern;
- *Practice Controls*: Promotion of changes in behavior (e.g., not pouring chemicals down the drain) to prevent emission and subsequent exposure to substances of concern;
- *Engineering Controls*: Implementation of new engineering processes (e.g., implementation of new water treatment processes in wastewater treatment plants) to prevent the emissions of the substance of concern;
- *Substitution*: Replacement of substances of concern in products or processes with chemical or non-chemical alternatives that are safer from a human health and environmental standpoint;

- *Elimination*: Phase-out of substances of concern from products or processes, without replacing them.

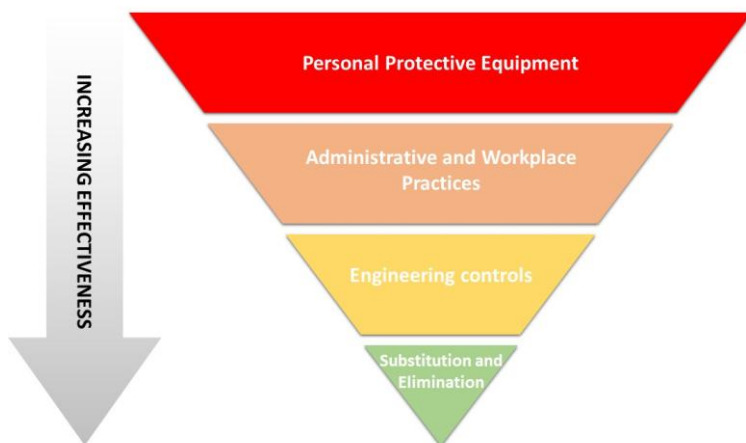


Figure 1. Risk management measures for better protection against harmful chemical substances (Inspired by Occupational Safety and Health Administration, 2024).

It is widely recognized that the substitution or elimination of substances of concern from products or processes is the most effective risk management measure, as this can prevent the exposure resulting from the use and disposal of the substance of concern while avoiding potential chemical accidents, equipment maintenance, etc. (Occupational Safety and Health Administration 2024).

### 1.3. Regulations to phase out the most harmful chemicals

Regulations on chemicals have entered into force over the past decades to control, restrict, or ban the uses of substances of concern to better protect human health and ecosystems. Existing chemical legislation can be divided into three categories based on the scope of the regulation (Government Offices of Sweden 2019):

- *Substances-oriented legislation*: Focus on predicting the risk to human health and the ecosystems posed by individual chemical substances or well-defined mixtures placed on the market for specific uses. Globally, examples include the Montreal Protocol, which addresses substances depleting the ozone layer (United Nations 2023b), and the Stockholm Convention, which addresses

persistent organic pollutants (POPs) (United Nations Environment Programme 2023). In the EU, examples of substances-oriented regulations include the regulations addressing cosmetic products (European Parliament 2009a), materials intended to come into contact with food (European Parliament 2004a), Plant Protection Products (European Parliament 2009b), medicinal products for human and veterinary use (European Parliament 2004b), and the Registration, Evaluation, Authorisation, and Restriction of Chemicals (REACH) Regulation (European Parliament 2006).

- *Emissions-oriented legislation:* Aim to limit emissions to the environment from industrial or waste management activities. The pollutants (or mixtures of pollutants) are not necessarily known, and the impacts of the pollution often depend on local factors influencing the application of the rules. In the EU, the Industrial Emissions Directive is the main legislation to regulate industrial emissions (European Parliament 2010).
- *Recipient-oriented legislation:* Aim to establish good environmental quality for a specific environmental compartment or recipient. The rules may focus on a specific set of pollutants/substances prioritized for action. An example of this type of legislation in the EU is the Water Framework Directive (European Parliament 2000).

This thesis focuses on the Stockholm Convention and the EU REACH Regulation as they cover the widest scope of chemical substances in terms of uses.

Entering into force in 2001, the Stockholm Convention is a global agreement aimed at protecting human health and the environment from POPs (United Nations Environment Programme 2023). POPs are substances that “remain intact for exceptionally long periods, become widely distributed throughout the environment as a result of natural processes involving soil, water, and, most notably, air, accumulate in living organisms including humans, [...] and are toxic for both humans and wildlife” (United Nations Environment Programme 2024b). Each Party to the Convention is required to: (1) Prohibit or eliminate the production and use of the substances listed in Annex A; (2) Restrict the production and use of the substances listed in Annex B; and (3) Reduce and eliminate releases of unintentionally produced substances listed in Annex C. As of November 2024, 30 substances are listed in Annex A, two substances are listed in Annex B, and seven substances are listed in Annex C (United Nations Environment Programme 2024a). A Party can nominate a substance to be listed in one of

the annexes of the Convention, which triggers a three-step scientific assessment by the POPs Review Committee (POPRC): (1) Screening of the properties of the substance of concern against the criteria listed in Annex D of the Convention to be considered a POP; (2) Assessment of the substance risk profile considering hazard and exposure in accordance with Annex E of the Convention; and (3) Risk management evaluation assessing the socio-economic aspects in accordance with Annex F of the Convention. Based on these assessment reports, POPRC develops recommendations on the potential listing (or not) of the substance of concern in annexes A, B, or C to the Conference of Parties (COP), the Convention's governance body. The COP takes the final decisions on the listing of the substance, including potential exemptions for specific uses (United Nations Environment Programme 2023).

At the EU level, the REACH Regulation came into force in June 2007 to “improve the protection of human health and the environment from the risks that can be posed by chemicals, while enhancing the competitiveness of the EU chemicals industry” (European Chemicals Agency 2023f). If the risk posed by a chemical substance is not properly managed, the authorities can restrict the use of the substance via the restriction and authorisation processes, among others (European Chemicals Agency 2023e; 2021b).

The restriction process can limit or ban the use of chemical substances that pose unacceptable risks to human health and/or the environment. It can be applied to any substance on its own, in a mixture, or in an article. The process can be initiated by a member state or by the European Commission, which commissions the European Chemicals Agency (ECHA) to prepare a restriction. Twelve months after the intention to propose a restriction is made public, the dossier submitter (i.e., the member state, or ECHA) must submit a restriction proposal containing background information on the identity of the substance of concern and justifications for the proposed restriction. It includes a description of the risks posed by the uses of the substances concerned by the restriction, any information on the availability of potential alternatives, and the costs and benefits for society resulting from the restriction. The restriction proposal is evaluated by the Committee for Risk Assessment (RAC) and the Committee for Socio-Economic Analysis (SEAC), which provide their opinion on whether the suggested restriction is appropriate to reduce the risks posed by the substance of concern, and on its socio-economic impacts, including potential derogations for specific uses. Based on RAC and SEAC opinions, the European Commission takes the final decision on the proposed restriction, including potential derogations (European Chemicals Agency 2023e).

The authorisation process aims to protect human health and the environment from substances of very high concern (SVHC) by facilitating their phase-out (European Chemicals Agency 2023f). The process is initiated by a member state or ECHA, at the request of the European Commission, by proposing a substance to be identified as SVHC. A substance may be considered SVHC if it meets the criteria to be classified as carcinogenic, mutagenic, or toxic to reproduction (CMR) category 1A or 1B under the EU Classification, Labelling, and Packaging (CLP) Regulation; it is persistent, bioaccumulative, and toxic (PBT) or very persistent and very bioaccumulative (vPvB) according to Annex XIII of REACH; or if it presents an equivalent level of concern, such as endocrine disruption (European Chemicals Agency 2024c). Once a substance is identified as SVHC, it is added to the Candidate List (European Chemicals Agency 2023d). ECHA regularly prioritizes substances to be included in the Authorisation List based on the information on their intrinsic properties, and whether the use is widespread and in high volumes in the EU. The Member State Committee prepares its opinion based on ECHA's recommendations for prioritization, and the European Commission takes the final decision to include a new SVHC in the Authorisation List (European Chemicals Agency 2024b). Once a substance is listed in the Authorisation List, the European Commission sets a sunset date, after which any uses of the substance in the EU are prohibited. If a company intends to keep using the substance after the sunset date, they must submit an application for authorisation (AfA) to ECHA in which they must demonstrate (1a) that the risk linked to their use of the SVHC is adequately controlled (the so-called "adequately controlled route"); or (1b) that the socio-economic benefits resulting from their use of the SVHC outweigh the risks (the so-called "SEA route"); and (2) that there are no suitable alternatives available for their particular use of the SVHC. RAC and SEAC evaluate the AfA and issue their opinion on whether a time-limited authorisation to keep using the SVHC is justified or not. The European Commission takes the final decision to grant the authorisation to the applicant or not (European Chemicals Agency 2024a).

Previous studies from ECHA have demonstrated that the REACH Regulation successfully enhances the substitution of substances of concern through its restriction and authorisation processes (European Chemicals Agency 2020b; 2021a). However, in its latest review of the REACH Regulation, the European Commission concluded that the authorisation process is too heavy and inflexible and that the restriction process is too slow to sufficiently protect professional and consumer users (European Commission 2018b; 2018a). To address these issues, the Commission wishes

to review both processes as part of the Chemical Strategy for Sustainability (CSS) (European Commission 2020). One of the proposed actions is to implement the “essential-use” concept to guide decision-making to phase out the uses of the most harmful chemicals (European Commission 2020).

#### 1.4. The “essential-use” concept

The “essential-use” concept was first introduced in 1987 in the Montreal Protocol to guide the phasing out of the uses of ozone layer-depleting substances (United Nations 2023b; 2023a). In Decision IV/25 adopted in 1992, the Parties agreed that all uses of the substances of concern should be banned, except for those uses that could be considered “essential”. They specified that a “controlled substance should qualify as “essential” only if: (1) it is necessary for health, safety, or is critical for the functioning of society (encompassing cultural and intellectual aspects); and (2) there are no available technically and economically feasible alternatives or substitutes that are acceptable from the standpoint of environment and health” (United Nations 2023a). In 2019, it was suggested that the concept could be implemented to guide the phasing-out of per- and polyfluoroalkyl substances (PFAS) by allowing their uses only if they are deemed “essential” (Cousins et al. 2019; 2021). As previously mentioned, the European Commission planned within the CSS to implement the “essential-use” concept to guide the phasing out of the uses of any substances that could cause “cancers, gene mutations, affect the reproductive or respiratory systems, or are persistent and bioaccumulative”, and substances that could affect “the immune, neurological or respiratory systems and [...] are toxic to specific organ”, so-called the “most harmful chemicals” (European Commission 2020).

Since the announcement of the CSS, work has been ongoing at the EU level to determine whether and how the “essential-use” concept could be implemented in the chemical regulations to guide the phasing-out of the uses of the most harmful chemicals (WSP Environment & Infrastructure Solutions et al. 2023). In April 2024, the European Commission published the first list of guiding criteria and principles for the implementation of the concept in EU regulations. Overall, they suggested that three main questions should be considered when evaluating the essentiality of a use: (1) Is the technical function of the most harmful substance needed for the final product to deliver its service? (2) Does the use of the most harmful substance fulfill at least one of the criteria listed in the guidance (Table 1 and 2) to be considered necessary for health and safety or critical for the functioning of society? (3) Are safer alternatives available that are capable of

providing a similar function and level of performance that society can accept? (European Commission 2024). Work is still needed to understand how the concept could be implemented in chemical regulations, such as REACH, to guide decision-making.

Table 1. Criteria for considering a use as "necessary for health and safety" (European Commission 2024).

Criteria	Additional information
<i>Preventing, monitoring or treating severe health issues</i>	<p>Uses may include those in medical devices, pharmaceuticals, healthcare, or other health-related uses, directly linked to the prevention, monitoring, or treatment of severe health issues.</p> <p>Mental illness should be included in "severe health issues" if patients affected by psychological problems have their abilities to engage in functional and occupational activities severely impaired.</p>
<i>Sustaining basic conditions for human life and health</i>	<p>"Basic conditions for human health and life" include food, water, and shelter/security. Environmental health can be included here (e.g. if used to prevent air pollution).</p>
<i>Managing and preventing health crises and emergencies</i>	<p>E.g. Human health disease outbreak.</p>
<i>Personal safety</i>	<p>Proper functioning of products/processes where the purpose of the chemical/product/process is to ensure personal safety (e.g. personal protection equipment, seatbelts, fire resistance products).</p>
<i>Public safety</i>	<p>Safety of public infrastructure (e.g. road safety, public building safety) as well as uses required to ensure the effective functioning of emergency services to prevent danger to public safety (which could include, for example, military, police, anti-terrorism, cyber security, and fire safety services).</p>
<i>Address a danger to animal health which cannot be contained by other means</i>	<p>Safeguarding animal health and welfare in line with EU standards; Prevention and control of diseases, and parasites; Prevention or minimisation of suffering caused to animals or pests, for example in the case of products used for pest control.</p>

Table 2. Criteria for considering a use as "Critical for the functioning of society" (European Commission 2024).

Criteria	Additional information
<i>Providing resources or services which are critical for society</i>	Meaning resources (e.g. raw materials) and services which must remain in service for society to function (e.g. critical infrastructure in energy and transport; waste treatments; water treatments; communication infrastructure; and healthcare infrastructure).
<i>Managing societal risks and impacts from natural and man-made crises and emergencies</i>	E.g. repairing/preventing damages to infrastructure in case of natural disaster.
<i>Protecting cultural heritage</i>	"Cultural heritage" can be understood as (i) monuments, (ii) groups of buildings, (iii) sites.
<i>Running traditional and religious practices</i>	Applied in a similar way as in the Minamata Convention.
<i>Protecting and restoring the natural environment</i>	E.g. To reduce emissions of greenhouse gases or biodiversity losses; for analysis and monitoring of pollutants; and for remediation of pollutants in the environment.

The European Commission suggests that the context of the use of the substance of concern should be properly defined before assessing its essentiality. To do so, it is important to identify the final product(s) or service(s) resulting from the use of the substance, assess the technical performance of the final product and how it is impacted by the technical function of the substance, and establish a set of requirements for the use or the final product that potential alternatives would need to fulfill (European Commission 2024).

A group of researchers suggested that the functional substitution approach could be a useful tool for linking the technical function of a chemical of concern with the performance of the final product (Roy et al. 2022). First described in 2015, the functional substitution approach suggests that three different function levels of a chemical substance should be defined when determining its use: the chemical function, the end-use function, and the function as a service (Table 3) (Tickner et al. 2015). By doing so, it is then possible to identify different types of alternatives to a substance of concern (e.g., alternative materials, products, technologies), and go beyond only considering "drop-in substitutes", i.e. alternative substances with a similar

molecular structure and similar physico-chemical property (Tickner et al. 2015). How the functional substitution approach could be implemented within the “essential-use” concept in practice still needs to be investigated.

Table 3. Definition of the different function levels of chemical substances (Tickner et al. 2015).

<b>Function level</b>	<b>Definition</b>	<b>Example with Bisphenol A use in thermal paper</b>
<i>Chemical function</i>	Also referred to as “technical function”, the chemical function is the actual technical function of the substance of concern, generally determined by its physico-chemical properties.	Color developer
<i>End-use function</i>	The end-use function specifies the specific purpose provided by the substance of concern in a product or process. In other words, what does the substance of concern bring to the product or process?	Creation of a printed image
<i>Function as a service</i>	The service relates to the broad service provided by the substance of concern in a product or process. In other words, what are the services provided by the specific end use of the substance of concern?	Record of a sale by printing cash receipts

### 1.5. Assessment of alternatives needed to avoid regrettable substitution

When eliminating the use of a substance of concern, a careful evaluation of the potential alternatives the substance could be replaced with is needed to avoid regrettable substitution (Occupational Safety and Health Administration 2024; Jacobs et al. 2016). Regrettable substitution occurs when a substance of concern is replaced by an alternative that is found to be of concern as well. For example, due to the regulatory efforts to restrict the uses of perfluorooctanoic acid (PFOA), its use in the manufacture of fluoropolymers was substituted with hexafluoropropylene oxide dimer acid (HFPO-DA), also known as GenX (Hopkins et al. 2018). However, there are now studies demonstrating that the concentrations of HFPO-DA in drinking water are increasing and that the substance is toxic to human health (Sun et al. 2016; Gebreab et al. 2020; Yang et al. 2022). Regrettable

substitution can also happen when the burden on human health or the environment is shifted from one endpoint to another. For instance, after the Montreal Protocol entered into force, the uses of chlorofluorocarbons (CFCs), which depleted the ozone layer, were substituted with hydrofluorocarbons (HFCs) (United Nations 2018; Falkner 2004; Prinn et al. 2000). It was later demonstrated that, although HFCs do not threaten the ozone layer, most of them have high global warming potential (Australian Government 2024). To address this concern, Parties to the Montreal Protocol agreed to amend the Treaty in 2016 to restrict the uses of HFCs with a high GWP (United Nations 2018). These substances were then substituted with other HFCs with a lower global warming potential and with hydrofluoroolefins (HFOs) which have a global warming potential significantly lower than HFCs (Holland et al. 2021; Papadimitriou et al. 2008). However, it was shown that several HFOs and HFCs degrade into trifluoroacetic acid (TFA) in the atmosphere (Holland et al. 2021; Behringer et al. 2021). Several studies have demonstrated that the concentrations of TFA in water (and other environmental media) are now increasing in several parts of the world (Holland et al. 2021; Behringer et al. 2021; Zhai et al. 2015; Pickard et al. 2020; Cahill 2022). Furthermore, TFA is already classified as acutely toxic, harmful to aquatic life with chronic effects, and corrosive to the skin (European Chemicals Agency 2024d), and Germany submitted a dossier to ECHA to classify it as toxic for reproduction, and as persistent, mobile, and toxic (PMT), and very persistent and very mobile (vPvM) (Garry 2024). Given the increase in the concentration of TFA in water and its potential toxic effects on human health, TFA is now raising concerns and actions to reduce its emissions should be taken (Arp et al. 2024).

Regrettable substitution could be avoided by conducting an assessment of alternatives. In short, this is a process that aims to identify, evaluate, compare, and select suitable alternatives to a substance of concern that are safer from the standpoint of human health and the environment (European Chemicals Agency 2021b). Different frameworks have been developed over the last decades to guide decision-makers in their alternative assessments. Although each framework is different, they contain similar components to structure the assessment (Jacobs et al. 2016).

### ***Identification of potential alternatives***

The first step of any assessment of alternatives is to identify potential alternatives to the substance of concern for the specific use of interest. Potential alternatives could be other substances or materials, but also alternative products, processes, or technologies that do not require the function provided by the substance of concern.

### ***Hazard characterization***

The hazard of the potential alternatives must be characterized with respect to their toxicological properties and their impacts on the environment. The number of endpoints and the level of detail of the hazard assessment may depend on the amount of data and the time available. Ideally, the hazard characterization should consider other environmental impacts (e.g., global warming potential, energy use, etc.) at different stages of the alternatives' life cycles (OECD 2021a). Although some studies have attempted to incorporate such elements in an alternative assessment (Fantke et al. 2020; Holmquist et al. 2021; 2020), more case studies are needed.

### ***Technical feasibility assessment***

This step aims to evaluate the purpose that a chemical performs or the properties that it delivers to a material or product. Other performance considerations such as quality, reliability, durability, and usability of the alternatives are also evaluated in the technical feasibility assessment (Jacobs et al. 2016; European Chemicals Agency. 2021).

### ***Economic feasibility assessment***

Direct and indirect costs of implementing the potential alternatives are evaluated to ensure that it is economically feasible to implement the alternative, and that the alternative would be able to penetrate the market (Jacobs et al. 2016).

### ***Comparison and selection of the alternatives***

Alternatives are compared with the substance of concern based on the hazard characterization, and technical and economic feasibility. The comparison can be performed simultaneously, i.e., all components are considered at the same time in the decision-making; or sequentially, e.g., the hazard characterization is considered first in the decision-making, then the technical feasibility, and the economic feasibility last (Jacobs et al. 2016).

Although substantial efforts have been made in the field of assessment of alternatives, more research is needed to address implementation gaps, in particular on the integration of life cycle considerations in the decision-making, and on the development of practical approaches to address trade-offs between safety, technical performance, and costs (Bechu et al. 2024).

## 1.6. Aim of the thesis

This thesis aims to investigate how the “essential-use” concept could be implemented in international and EU legislation. This includes determining the type of information needed for a proper essentiality assessment and evaluating how the “essential-use” concept differs from current regulatory practices, including potential implications of the implementation.

**Paper I** investigates how the functional substitution approach can be applied to determine the functions provided by PFAS across all their uses. It also aims to provide an overview of the availability of potentially suitable alternatives capable of providing similar functions.

**Paper II** investigates how the functional substitution approach and the “essential-use” concept could be applied in practice by taking the example of PMT substances used in cosmetic products. After evaluating whether the functions provided by PMT substances are necessary for the end-products, the study identifies, evaluates, and compares chemical alternatives to PMT substances to determine whether safer alternatives are available.

**Paper III** evaluate and compares non-chemical alternatives to a substance of concern by taking the example of PFAS used in insulation materials. Here, the method from **Paper II** is used to evaluate and compare other types of alternatives based on alternative criteria.

**Paper IV** investigates how the decision-making following the “essential-use” concept would differ from previous decisions made in current chemical legislation by taking the example of the Stockholm Convention and the REACH Regulation, including potential implications, to guide the decision-making to phase out the most harmful chemicals. The restriction on intentionally added microplastics under REACH was used to determine whether the “essential-use” concept could have been applied based on the information available to the authorities.

## 2. Methods

The “essential-use” concept was applied to examples of uses of various substances following the approach described in previous studies and by the European Commission (Figure 2) (Cousins et al. 2019; Roy et al. 2022; WSP Environment & Infrastructure Solutions et al. 2023; European Commission 2024). The following will provide an overview of the method followed for each step of the assessment.

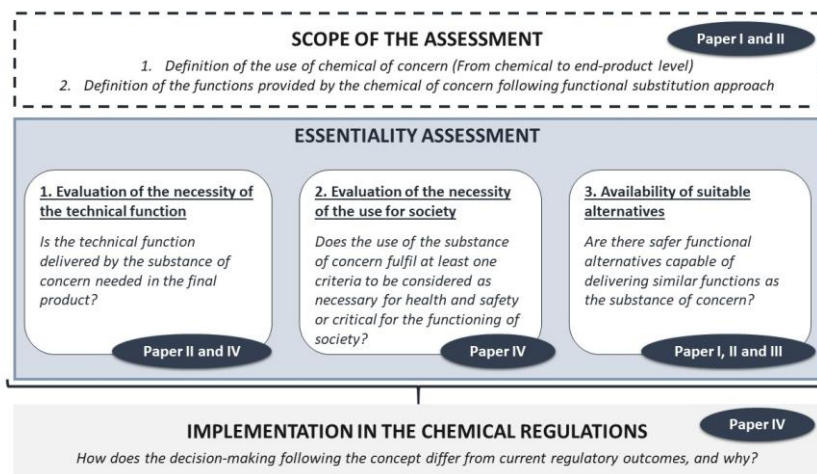


Figure 2. Overview of the approach taken to investigate the implementation of the “essential-use” concept.

### 2.1. Substances of interest

The methods developed as part of this project were applied to the uses of PFAS (**Paper I; Paper III**) and PMT substances (**Paper II**) as these groups of substances could be considered as the “*most harmful chemicals*” as described in the CSS. PFAS are defined as any substance containing a fully fluorinated methyl ( $-\text{CF}_3$ ) or methylene ( $-\text{CF}_2-$ ) group in its molecular structure, as proposed by the Organisation for Economic Co-operation and Development (OECD) (OECD 2021b). PMTs are substances defined as persistent and toxic according to Annex XIII of the REACH Regulation, and which have a logarithm of the organic carbon-water partition coefficient ( $\log K_{oc}$ ) lower than 4, as recommended by the German Environment Agency (Arp and Hale 2019).

For the purpose of this work, “microplastics” were defined as a material consisting of solid polymer-containing particles, to which additives or other substances may have been added, where at least 1% w/w of particles

have a dimension between 1 nm and 5 mm, or for fibers a length between 3 nm and 15 mm and a length to diameter ratio greater than 3, as defined in the restriction proposal (European Chemicals Agency 2019) (**Paper IV**).

## 2.2. Definition of the use of a substance and its functions following the functional substitution approach

For groups of substances for which a restriction proposal has been submitted under REACH, the uses were identified based on the information collected by the dossier submitters (European Chemicals Agency 2023c; 2023a; 2019; 2020a). The chemical functions delivered by the substances in each identified use were determined following the OECD guidance on harmonized classification of uses of chemicals based on the information available in the respective restriction proposals (OECD 2017). The end-uses and services delivered by the substances were defined by a careful examination of the tasks a chemical, product, or technology is intended to fulfill in each use case (**Paper I, Paper III, Paper IV**).

For the specific case of PMT substances used in cosmetic products, substances listed in the database of cosmetic ingredients (CosIng) of the European Commission (European Commission 2023) that satisfy the PMT definition were identified using the list of PMT substances registered under REACH published by the German Environment Agency (Arp and Hale 2019). The Danish Consumer Council Think Chemicals and Cosmetics databases were then screened to determine the types of cosmetic products PMT substances are used in. Their chemical functions were determined based on the information provided in the Cosing database. The end-use functions and services provided in each type of cosmetic product were defined based on interviews with representatives of the cosmetic industry (**Paper II**).

## 2.3. Evaluation of the necessity of the use of the substance of concern for the final end-product

The necessity of the use of the substance for the technical performance of the end-product was determined based on the information collected on the chemical functions, end-use functions, and services provided by the substances of concern, by comparing those functions with the intended purpose of the end-product (**Paper II, Paper IV**).

## 2.4. Evaluation of the necessity of the use of the substance of concern for society

The necessity of the use of the substances of concern for health and safety, and for the functioning of society was evaluated by assessing whether the functions delivered by the substances of concern would satisfy at least one of the criteria proposed by the European Commission (European Commission 2024) (Tables 1 and 2) (**Paper IV**).

## 2.5. Evaluation of the availability of suitable alternatives

The ECHA framework on assessment of alternatives was followed to determine whether suitable alternatives to the substances of concern were available (European Chemicals Agency 2021b). Although the approach was similar in the different studies, the exact methods used for each component of the assessment of alternatives differed. Table 4 summarizes the different methods used for each study.

Table 4. Summary of the different methods followed to evaluate the alternatives in the different case studies.

Case study	Type of alternatives	Identification of alternatives	Evaluation of hazard	Evaluation of technical performance	Economic feasibility	Comparison of alternatives
<i>Multi-uses of PFAS (Paper I)</i>	Substances Materials Products Processes Technologies	- Analysis of the restriction proposals (European Chemicals Agency 2023b; 2022) - ChemSec webtool MarketPlace (ChemSec 2023)	Screening of potential concerns using the SUBSPORT Plus database (Bundesanstalt für Arbeitsschutz und Arbeitsmedizin (BAuA) 2023)	Qualitative evaluation	Qualitative evaluation	Semi-sequential and qualitative comparison
<i>PMT substances used in cosmetic products (Paper II)</i>	Substances	Use of the CosIng database (European Commission 2023)	Full hazard characterization	Not evaluated	Not evaluated	Simultaneous quantitative comparisons
<i>PFAS used in insulation materials (Paper III)</i>	Materials	Use of the alternatives to the PFAS database Semi-structured literature review	Life cycle assessment	Semi-structured literature review	Not evaluated	Simultaneous and sequential quantitative comparison

## 2.6. Implementation of the “essential-use” concept in chemical legislation

Following the READ approach, a method for the systematic analysis of policy documents (Dalglish, Khalid, and McMahon 2020), the rationale behind existing restriction outcomes under REACH was analyzed. Specifically, a review of the opinions adopted by SEAC to ECHA on the proposals for restrictions compared to the final legal text adopted by the European Commission was conducted. This was done to determine the main reason for granting a specific derogation (e.g., critical for health, safety, or the functioning of society; a lack of alternatives; time needed for transition; etc.). A similar analysis of the risk management evaluations from the POPRC compared to the final decision by the COP under the Stockholm Convention was performed (**Paper IV**). Table 5 summarizes how the READ approach was implemented for this analysis.

An evaluation of previous decisions on applications for authorisation was also performed to determine the reasoning for granting authorisations under the REACH Authorisation process. The REACH restriction dossier on intentionally added microplastics served as a case study to assess how the implementation of the concept may influence restriction outcomes based on the information presented in the restriction proposal (**Paper IV**).

Table 5. Summary of the READ approach followed for the analysis of policy documents (*Paper IV*).

Regulation	Step 1: Readyng the material	Step 2: Extraction of the data	Step 3: Analysis of the data	Step 4: Distilling the findings
<i>Stockholm Convention</i>	POPRC Risk management evaluation ( <i>n</i> = 22) Decision of the COP ( <i>n</i> = 22)	Information on the rationale of POPRC for recommending exemptions, and final decision by COP.	Exemptions are grouped into 4 categories based on the main reason for recommending it: (1) referring to the necessity of the technical function for the performance of the end-product; (2) referring to the necessity of the use for health and safety, or its criticality for the functioning of society; (3) referring to the lack of suitable alternatives is mentioned; and (4) referring to other reasons (e.g., negligible releases/exposure/risks, the chemical(s) present as impurities in other products, costs outweigh the benefits)	The data were analysed to determine how the outcomes of the Stockholm Convention match or differ from the essential-use concept.
<i>REACH Regulation – Restriction process</i>	SEAC final opinions ( <i>n</i> = 45) Legal decision of the European Commission ( <i>n</i> = 29)	Information on the rationale of SEAC for recommending derogations, and final decision by the European Commission.		The data were analysed to determine how the outcomes of the Restriction process under REACH match or differ from the essential-use concept.

## 3. Results and Discussion

### 3.1. Uses and functions of the substances of concern

Overall, 325 different applications of PFAS were identified across 18 use categories based on the information collected in the restriction proposal. By following the functional substitution approach, it was estimated that PFAS delivered 39 different chemical functions, 131 end-use functions, and 201 services across the identified application. Furthermore, PFAS deliver more than one function in the majority of the identified applications (**Paper I**).

Regarding PMT substances, 50 substances satisfying the PMT criteria proposed by the German Environment Agency are listed in the CosIng database. Based on information from the Cosmetics and Kemiluppen databases, 21 substances were identified as being used in cosmetic products available on the EU market. Based on their high occurrence in cosmetic products, Allura Red (CAS: 25956-17-6), Benzophenone-4 (CAS: 4065-45-6), and Climbazole (CAS: 38083-17-9) were selected as case study chemicals for the assessment. Their chemical functions, end-use functions, and services are listed in Table 6 (**Paper II**).

Based on the information collected in the restriction proposal on intentionally added microplastics, 23 applications of microplastics were identified across 10 different product categories. Qualitative information regarding the chemical functions, end-use functions, and services they provide was collected for 18 applications based on the information in the restriction proposal. Microplastics deliver more than one function for the majority of these applications (**Paper IV**).

### 3.2. Evaluation of the necessity of the use of a substance of concern for the final end-product

Interviews with representatives from the cosmetic industry helped evaluate whether the functions provided by the case study PMT chemicals are necessary for the technical performance of the end-product. If the functions were considered unnecessary, the substance would then be considered “not fit-for-purpose” in the specific use as suggested by Roy *et al.* (2022), meaning it could be phased out without being replaced by an alternative, as the use would be considered non-essential (**Paper II**). For example, a red pigment could be considered “fit-for-purpose” if used in

red lipstick, as the lipstick would lose its primary purpose without the pigment. However, the same red pigment is not “fit-for-purpose” if used in soap as the soap would perform just as well to clean the body without it (**Paper II**). Table 6 summarizes the “fit-for-purpose” assessment for the case study of PMT substances used in cosmetic products.

Table 6. "Fit-for-purpose" assessment of case study of PMT substances used in cosmetic products (**Paper II**).

Substance of concern	Type of product	Chemical function	End-use function	Service	Is it “fit-for-purpose”?
<i>Allura Red</i> (CAS 25956-17-6)	Make-up; Hair color products	Pigment	Provide a color to the formulation	Change the appearance of certain body parts	<b>YES</b>
	Soap; Tooth-paste	Pigment	Provide a color to the formulation	Improve consumer perception of the product	<b>NO</b>
<i>Benzophenone-4</i> (CAS 4065-45-6)	Sun care products	UV-filter	Protection of a surface against sunlight	Protect the consumer from the sun	<b>YES</b>
	Other types of cosmetic products (e.g. cream)	UV-filter	Protection of the formulation against sunlight	Increase the shelf-life of the product	<b>YES</b>
<i>Climbazole</i> (CAS 38083-17-9)	Anti-dandruff shampoo	Anti-seborrheic agent	Provide anti-seborrheic properties to the product	Treat against seborrheic dermatitis	<b>YES</b>

A similar approach was taken to evaluate the “fitness-for-purpose” of microplastics. Overall, the use of microplastics was considered “fit-for-purpose” for 15 out of the 18 applications evaluated. In some cases, not all functions provided by microplastics in a single application were deemed necessary for the end product. For instance, microplastics are used in detergents as rheology modifiers, anti-foaming agents, and/or complexing agents, but also as opacifiers. While the former functions are necessary for a detergent to perform well, as they improve the efficacy of the detergent function, opacifiers are only used to provide a “milky texture” to the product, enhancing consumer perception without contributing to the technical performance of the detergent. Although the use of microplastics in detergents can be considered “fit-for-purpose” overall, the essentiality assessment should focus only on the functions necessary for the performance of the end product, especially when identifying alternatives (**Paper IV**). Further work is needed to similarly evaluate the functions provided by PFAS in identified applications to determine if they are necessary for the optimal performance of the end products they are used in (**Paper I**).

To the best of my knowledge, no standardized methods have been proposed to evaluate the “fitness-for-purpose” of a chemical substance. One option could be to define a functional unit, as done in the context of a life cycle assessment (LCA). Defined as “*a measure of performance of the functional outputs of a product system*”, the functional unit aims to provide a reference to ensure that different alternatives are compared on a common basis in an LCA (Cooper 2003). The information on the different function levels of a substance of concern collected by following the functional substitution approach could be used to define such a functional unit. For the specific case of PFAS used as foam blowing agents in insulation materials, a functional unit was defined as the volume of insulation material corresponding to an area of 1 m<sup>2</sup> with a thermal transmittance of 1 W/m<sup>2</sup>K, the reference value generally used to evaluate insulation materials (Füchsl, Rheude, and Röder 2022). This functional unit was used to compare the different functional alternatives (**Paper III**). As LCA is a standardized method (ISO 14040:2006) (International Standards Organization 2006) that has been implemented in various concrete case studies over the past decades, lessons learned from this field of research could be useful when developing a standardized method for evaluating the “fitness-for-purpose” of a substance of concern as part of an essentiality assessment.

### 3.3. Evaluation of the necessity for health and safety, and the criticality for the functioning of society

Once the purpose of the substance of concern in a specific end-product or process is properly defined, it becomes possible to evaluate whether the service provided by the substance in the context of the end product is necessary for health and safety, or critical for the functioning of society. Such an assessment was performed on the specific case of intentionally added microplastics based on the information provided in the restriction proposal (European Chemicals Agency 2020a; 2019). Out of the 23 applications assessed, the uses of microplastics were considered necessary for health and safety and/or critical for the functioning of society in ten cases, where it was very clear that the functions delivered by microplastics comply with at least one of the criteria listed by the European Commission (Table 1; Table 2). For instance, microplastics are used in *in-vitro* diagnosis (IVD) kits as carriers for reagents, calibrators, or purification agents, all necessary for immunoassays, which are used to “*prevent, monitor, or treat severe health issues*”. However, in some cases, no conclusions could be reached because not enough detailed information regarding the end product was available. For instance, microplastics are used in paints and coatings to provide friction resistance and anti-slip effects. These functions could be considered necessary for health and safety, or critical for the functioning of society if used in road marking, but not if used in paints for decorative purposes (**Paper IV**).

Although the criteria listed by the European Commission provide a good basis for such an assessment, more work is needed to properly evaluate the necessity of the use of a substance for society. In particular, determining whether the use of a substance is “critical for the functioning of society” requires a broader consideration of societal values, beliefs, and preferences, implying a greater involvement of various interested parties (Suffill et al. 2024). Such an assessment requires a transdisciplinary approach involving social and behavioral scientists. Further work is needed to investigate how “social data” could be incorporated into the decision-making to evaluate the essentiality of a use of a chemical.

### 3.4. Availability of suitable alternatives

#### 3.4.1. Identification of potential functional alternatives

For Allura Red, Benzophenone-4, and Climbazole, 47, 39, and 10 potential chemical alternatives, respectively, were identified in the CosIng database based on the chemical functions they provide to the cosmetic products (**Paper II**).

Various types of alternatives to a substance of concern for a specific use could be identified based on the information on the different function levels collected by following the functional substitution approach. For instance, alternative substances and materials to PFAS used as foam-blowing agents in insulation materials could be identified for the different function levels. In short, fluorinated gases are used in rigid polyurethane (PU) and extruded polystyrene (XPS) foams as *foamants* for their capacity to ensure the good expansion of the foam. These foams are then used in buildings as insulation materials (**Paper I**, Figure 3).

When identifying potential alternatives, one could aim to find substitutes capable of ensuring the expansion of the PU and XPS foams, such as alternative foam blowing agents (e.g., pentane; methyl formate). Another strategy could be to look for alternative insulation materials that do not require the use of a foam-blowing agent to replace PU and XPS foams for the insulation of a building. In total, 7 alternative blowing agents and 53 alternative materials were identified (**Paper III**, Figure 3).

Overall, a total of 162 chemical alternatives, 163 alternative materials, 128 alternative products, 37 alternative processes, and 40 alternative technologies to PFAS were identified across the 325 applications of interest (**Paper I**).

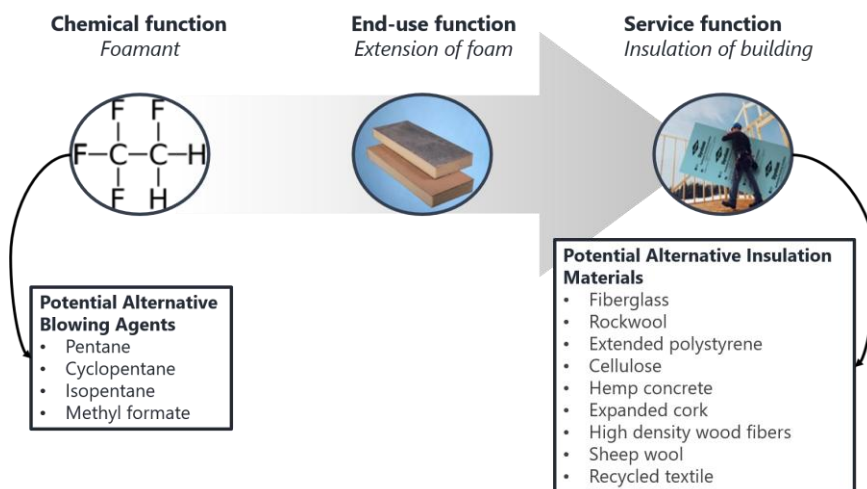


Figure 3. Identification of potential alternatives to fluorinated gases used in insulation materials according to the functional level being considered.

### 3.4.2. Evaluation of the functional alternatives

#### *Safety considerations*

The SubsPort Plus database (Bundesanstalt für Arbeitsschutz und Arbeitsmedizin (BAuA) 2023) was used to determine whether potential concerns regarding alternatives to PFAS were already identified by different stakeholders (i.e., governmental authorities, companies, or non-governmental organizations). Out of the 198 alternatives for which such evaluation could be performed, concerns were identified in 68 of them. Overall, alternatives without presently identified concerns were found for 142 applications of PFAS (**Paper I**).

A similar approach was taken to shortlist the potential chemical alternatives to Allura Red, Benzophenone-4, and Climbazole. After the shortlisting, 6, 6, and 5 chemical alternatives, respectively, not listed in the SubsPort Plus database were selected for further evaluation. Data were then collected for 26 different endpoints to evaluate the environmental degradation, bioaccumulation potential, mobility, and toxicity to human health and the environment of the shortlisted alternatives (**Paper II**).

For non-chemical alternatives, such an approach may be difficult as it would require properly identifying and evaluating the potential adverse effects of all the constituents of an alternative product, material, process,

or technology, taking into account any potential mixture effects between the constituents. To address this issue, alternative materials to PFAS used in insulation materials were evaluated based on LCA results. Data related to the impacts on climate, ozone layer depletion potential, other environmental impacts, ecotoxicity, human toxicity, and resource use were collected for 9 shortlisted insulation materials that do not require the use of fluorinated gases (**Paper III**).

### ***Technical feasibility***

All shortlisted alternatives to Allura Red, Benzophenone-4, and Climazole were considered technically feasible as they can deliver the same technical function as the substances of concern. No assessment of the difficulty of using them in cosmetic products was performed, as it is highly dependent on the specific formulations of the products, and it could not be generalized (**Paper II**).

Based on the information collected in the restriction proposal, it was considered that 259 potential alternatives to PFAS were capable of providing similar or greater technical performance than the substances of concern. 231 of the alternatives provide satisfactory performance but only for a limited range of environmental conditions, and only for a limited number of functions of interest. More tests were needed at the time of the study for 29 potential alternatives to ensure they could provide satisfactory technical performance to replace PFAS (**Paper I**).

For the specific use case of PFAS as blowing agents in insulation foams, the technical performance of alternative insulation materials was evaluated based on their thermal insulation, humidity insulation, and fire resistance. Data related to these criteria were collected for all 9 shortlisted insulation materials (**Paper III**).

### ***Economic feasibility***

The economic feasibility is difficult to evaluate as it depends on the actor trying to implement the alternative. As an approximation, it was considered that any alternatives to PFAS that were already available on the market and in use at the time of the study were considered economically feasible. Based on the information in the restriction proposal, 305 identified alternatives could be considered economically feasible. 144 alternatives were already available on the market but in use for only a limited number of applications. 58 identified alternatives were still at the patent stage or the testing phase at the time of the study and were not considered economically feasible (**Paper I**).

### 3.4.3. Comparison and selection of functional alternatives

Potential alternatives to PFAS were compared qualitatively by first evaluating their suitability based on the information collected on performance loss and market availability. It was estimated that suitable alternatives are available for 40 applications of PFAS, out of the 325 applications evaluated. By adding safety considerations to the decision-making, suitable alternatives without presently identified concerns could be identified for 28 applications of PFAS. This provides a general overview of the substitution potential of PFAS across their multiple uses, and further assessment of the alternatives is needed (**Paper I**).

Shortlisted alternatives to Allura Red, Benzophenone-4, and Climbazole were compared using three different multicriteria decision analysis (MCDA) methods. At least one alternative that consistently ranked better than the substances of concern using the different MCDA methods could be identified for all three case study chemicals (**Paper II**).

The multi-attributes utility theory (MAUT) was adapted to compare alternative insulation materials to PFAS used as blowing agents in insulation foams based on technical performance criteria, and LCA results. The MAUT approach was considered the most appropriate method as it is easy to implement, while still allowing good flexibility, and transparency to describe the choices made to justify the final ranking of alternatives. Alternatives that consistently ranked better than materials containing PFAS could be identified in each decision-making scenario defined (**Paper III**).

### 3.5. Implementation of the “essential-use” concept in the chemical legislation

Overall, the analysis of the argumentation to justify granting derogations to previous restrictions under the Stockholm Convention and REACH suggests that the authorities can obtain the relevant information to perform an essentiality assessment. In other words, no fundamental changes in the regulatory processes are needed to implement the “essential-use” concept to guide decision-making. The concept brings the opportunity to shift the focus of the evaluation for a potential derogation on the actual functions provided by a substance of concern and the services delivered by the end products, and not on the relative risk posed by the specific use. For instance, in the case of the restriction on intentionally added microplastics, three derogations were proposed for uses believed to have controlled emissions of microplastics. Such cases would not have been discussed if the “essential-use” concept had been implemented at the time. Furthermore, four derogations were proposed for uses of microplastics in cosmetic products because suitable alternatives were not available at the time of the restriction proposal. Such derogations would not have been proposed if the “essential-use” concept had been implemented at the time, as the technical function provided by microplastics is not necessary for the technical performance of the final product and/or because the uses of microplastics in those particular products are not considered necessary for health and safety, nor critical for the functioning of society according to the criteria listed by the European Commission. Therefore, authorities could have quickly concluded that such derogations were not needed because those uses of microplastics are not essential, without trying to determine whether suitable alternatives are available or not (**Paper IV**).

In some cases, the competent authorities do not have comprehensive information on the whole value chain of a substance of concern to properly link the chemical functions of the substance with the services provided by the end products, which may hamper the essentiality assessment. To address this challenge, competent authorities could ask companies to clarify this point in a request for a time-limited derogation to a potential ban on the uses of the substance of concern they are using, as it is done under the REACH Authorisation process (**Paper IV**). However, in the current state of the Authorisation process, although companies are expected to provide all the relevant information for an essentiality assessment in their applications for authorisation (Figuière et al. 2023), a recent study demonstrated that for the majority of the applications submitted to ECHA, the information provided by the applicant is not clear enough to reach a conclusion

on the essentiality of the use applied for (Borchert et al. 2024). Further work is needed to investigate the quantity and type of information that competent authorities should request from companies to ensure that the implementation of the “essential-use” concept in the decision-making would make regulatory processes more efficient and less time-consuming.

Furthermore, as mentioned above, a use can be considered essential if no suitable alternatives are available from a societal perspective. More work is needed to determine who should be responsible for evaluating the availability of alternatives. One could argue that the assessment would be biased if companies were responsible, as they might not consider alternatives that do not require the functions provided by the substance of concern they are using. If the competent authorities are responsible for such evaluation, the essentiality assessment may become time- and resource-intensive, which would be against the main goal of implementing the “essential-use” concept in chemical regulations to make the decision making process more efficient (**Paper IV**).

## 4. Conclusions and Perspectives

Table 7 summarizes the number of non-essential uses of the substances of interest identified in this work. The results suggest that identifying non-essential uses of substances of concern is easier than identifying the essential uses. Since three non-negotiable conditions must be met for a use to be deemed “essential”, the assessment can be stopped as soon as one of the requirements is not fulfilled. This approach could speed up the decision-making process in a regulatory context.

From the analysis of the Stockholm Convention, and the Authorisation and Restriction processes under REACH, it appears no changes are needed in regulatory processes to implement the “essential-use” concept. The results indicate that authorities already have the capacity to gather the relevant information needed to determine if a use is (non-)essential. The “essential-use” concept is a promising tool that can help reduce the number of potential exemptions for uses of chemicals of concern. It also brings the opportunity to shift the focus of the decision-making, moving towards determining the true purpose a substance serves in the final product and to society, rather than the relative risks posed by its uses. However, to implement the “essential-use” concept effectively, it is crucial to properly understand how the chemical functions provided by the substance of concern are linked to the services in the final products (i.e., what they provide to society), which requires cooperation with the industry throughout the value chain.

The availability of suitable alternatives is a crucial aspect of an essentiality assessment. Based on the case study chemicals from this work, the availability of suitable and safer alternatives was the main reason for classifying a use as “non-essential”. Although significant progress has been made in the field of assessment of alternatives, more work is needed to clearly define what “availability of suitable alternatives” means in an essentiality assessment, particularly in a regulatory context (e.g., Available to whom? Suitable for what purpose?). This work used the functional substitution approach, which provided a solid framework for understanding how the technical functions provided by a substance of concern are linked to the services it offers society. This information helps identify all potential alternatives relevant at the societal level, which is the most appropriate scope for an essentiality assessment in a regulatory context. In other words, a use of a substance of concern should not be considered essential if suitable alternatives of the specific substance are available, even if no suitable chemical

alternatives can be identified. More work is needed to develop proper guidance to identify relevant alternatives according to the functional substitution approach in a regulatory context.

This work explored how to implement the “essential-use” concept to phase out the uses of the most harmful chemicals. Another possibility is to apply the concept during the product design phase, limiting the formulation to only the components necessary for the product to deliver its intended service to society. The “essential-use” concept could be combined with the Safe and Sustainable by Design framework as an initial screening step to design new chemicals or materials only for the functions needed for the technical performance of the final product. Further research should explore how these two approaches could be integrated.

Lastly, the “essential-use” concept was first introduced to control substances depleting the ozone layer. This work examined how it could be implemented to control uses of the most harmful chemicals with the ultimate goal of tackling chemical pollution, potentially addressing the issue posed by the planetary boundary on novel entities. Further research could investigate how the “essential-use” concept might be applied to other planetary boundaries. For instance, the concept could be adapted to control the use of fossil fuels, aiming to decrease emissions of greenhouse gases, and to reduce the impact of human society on climate change.

Table 7. Number of non-essential uses for each substance of concern.

Substance of concern	Number of uses evaluated	Number of uses not “fit-for-purpose”	Number uses not necessary for society	Number uses for which suitable and safer alternatives are available
PFAS (Paper I and III)	325	Not assessed	Not assessed	28
Allura Red (Paper II)	2	1	Not assessed	1
Benzophenone-4 (Paper II)	2	0	Not assessed	2
Climbazole (Paper II)	1	0	Not assessed	1
Microplastics (Paper IV)	23	2	3	7

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