Journal of Cleaner Production 484 (2024) 144011

Contents lists available at ScienceDirect

Journal of Cleaner Production

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

Green chemistry and responsible research and innovation: Moving beyond the 12 principles

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ARTICLE INFO

Handling Editor: Xin Tong

Keywords:
Circular economy
Green chemistry
Responsible research and innovation
Responsible roadmapping
SDGs

ABSTRACT

Green chemistry focuses on designing products and processes that minimize hazardous substances and address pollution, resource depletion, and climate change. Green chemistry products and processes could contribute to the transition to circular economy and reaching Sustainable Development Goals. However, green chemistry philosophy offers none or little guidance on social, ethical, economic, or political aspects that are inherent to complex transition processes. Such broad and future-oriented considerations are at the heart of 'Responsible Research and Innovation' (RRI) approach but to date the ideas of RRI and green chemistry remain largely unconnected. This study aims to shed light on how RRI and green chemistry approaches can be combined. A refined responsible roadmapping method is proposed to help researchers to go beyond the 12 principles of green chemistry and develop inter- and transdisciplinary research agendas that address technical, environmental as well as social, ethical, economic and political considerations. The method was piloted in three research projects aspiring to develop sustainable and safe chemical processes and their applications. The study demonstrates that at the early stage of research planning, the responsible roadmapping method can facilitate the integration of RRI and green chemistry practices and the development of interdisciplinary research plans, which address technical, environmental, socio-ethical, economic and political dimensions. The implications of our study for future research on roadmapping methods as well as for policy and innovation practice are discussed.

1. Introduction

Chemical products and processes could play a key role in enabling transition to more sustainable production modes (Horváth and Anastas, 2007a) across industrial sectors, e.g., construction, manufacturing, public utilities, to mention just a few. Such advancements can contribute substantially to meeting the United Nations' Sustainable Development Goals (SDGs) (Chen et al., 2020; Garcia Martinez, 2016). However, "more than 98 % of all organic chemicals are still derived from petroleum" (American Chemical Society, 2024b) and many are hazardous (Martin et al., 2009). Hence, green chemistry is seen as a framework for advancing sustainable future (Ganesh et al., 2021). It aspires to design, develop, and implement chemical products and processes that reduce or eliminate the use and generation of hazardous substances (Anastas and Williamson, 1996; Manley et al., 2008). Its aim is to promote environmental and human health while preserving natural resources and fostering economic viability (Anastas and Eghbali, 2010; Horváth and Anastas, 2007b; Manley et al., 2008). It promotes innovative solutions that address the challenges of pollution, resource depletion, and climate change (Anastas and Eghbali, 2010; Anastas and Williamson, 1996; Horváth and Anastas, 2007a, 2007b).

To realise the aforementioned ambition of creating sustainable production modes and contributing to the SDGs with green chemistry, new technologies would need to be developed and embedded in complex socio-political-economic systems in a way that is beneficial for the people, planet, and prosperity. It is therefore essential that the

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https://doi.org/10.1016/j.jclepro.2024.144011
Received 25 July 2024; Received in revised form 3 October 2024; Accepted 15 October 2024

development and diffusion of green chemistry products and processes is accompanied by thorough consideration for ethical, social, political, legal and economic aspects. For instance, careful attention must be given to the unintended consequences.

Some scholars could turn for guidance to the widely cited 12 principles of green chemistry (American Chemical Society, 2024a). These principles guide the process of making the input and output streams more environment-friendly and "only the principles no. 4 (designing safer chemicals), no. 7 ([use of] renewable feedstock[s]), and no. 10 (design for degradation) go beyond" (Falcone and Hiete, 2019, p. 67). There is however no consensus on the number of principles required for a molecule or process to be deemed 'green' or on how to prioritise these principles (United Nations Environment Programme, 2019). The 12 principles offer also little to none guidance for addressing socio-ethical, political, legal and economic aspects related to the development and diffusion of green chemistry products and processes.

Frameworks such as 'sustainable chemistry' (Blum et al., 2017) and 'safe and sustainable by design' (Abbate et al., 2024; Caldeira et al., 2022) have been developed to take environmental, social, and economic dimensions into account (United Nations Environment Programme, 2019). However, the socio-economic assessment is optional in the application of 'safe and sustainable by design' according to the methodological guidelines provided by the European Commission (Abbate et al., 2024). Consequently, social and economic dimensions are often neglected. Social and economic sustainability assessments were conducted in less than a third of the research projects, while hazard, safety, and human health assessments were conducted in more than half of them, as reported by the surveyed partners of the Partnership for the Assessment of Risks from Chemicals (PARC) program (Leso et al., 2024). Therefore, other frameworks are still needed to ensure green chemistry research and innovation can contribute to sustainable industrial transitions considering technical, environmental as well as social, ethical, economic and political considerations. The Responsible Research and Innovation (RRI) framework is proposed here as promising alternative.

It has been recently argued that the RRI framework offers a promising approach to integrate "ethics dimensions" into "chemists' scientific practices" and it was suggested that also green chemistry could benefit from it (Mehlich, 2023, p. 12). RRI can provide a more holistic approach for integrating societal values, ethical considerations into green chemistry practices, and addressing the needs of different stakeholders throughout the entire R&D process. Mehlich (2023) highlights the value of combining green chemistry and RRI, but notes that there is a lack of understanding on how RRI principles can be incorporated in green chemistry practice besides the suggested educational initiatives (e.g., interdisciplinary collaboration and communication training for chemistry researchers). This study aims to address this challenge.

To date, the scientific discourses on green chemistry and RRI remain mostly disconnected (Mehlich, 2023) and it is unclear how RRI as a process-oriented approach can be embedded in R&D activities in the field of green chemistry. This study contributes to connecting the concepts of green chemistry and RRI while aiming to promote sustainable development and contribute to the SDGs. The novelty of this study is to deepen the understanding on *how the principles of RRI can be embedded in the development of green chemistry products and processes*. To address this question, we propose a responsible roadmapping method and analyse the application of the method in three green chemistry research projects aiming to contribute to circular economy. By this means, this study contributes to the literature in three ways. First, it highlights the need for green chemistry to go beyond the in-depth considerations of environmental and human health issues and pay more attention to socio-ethical, policy, and economic issues. Second, it is the first attempt to thoroughly investigate how RRI principles can be brought into green chemistry practice while RRI enjoys broad application in other fields (e.g., nanotechnology, biotechnology (Thapa et al., 2019)). Third, it illustrates how roadmapping processes can be adapted to embed the RRI principles into the planning of R&D activities and commercialisation of new technologies.

The remainder of the study is structured as follows: In Section 2 we will link the approaches of green chemistry and circular economy, discuss the concept of RRI and the challenges of embedding RRI principles in everyday R&D practice. Section 3 sets out the methodology. Section 4 presents three exploratory cases. The implications of the results for research and practice are discussed in section 5. Finally, Section 6 concludes the paper summarising its core contribution.

2. Theoretical background

2.1. *Green chemistry and circular economy*

Linder (2017) argues that the green chemistry approach could notably contribute to circular economy transitions, particularly through "the [green chemistry] principles [no. 1] prevent waste, [no. 2] optimize atom economy, [no. 3] use non-hazardous components, [no. 7] use renewable feedstocks, [no. 10] design for degradation" (p. 429). Furthermore, "[t]he limitation of hazardous chemical substances in the cycle of materials is not only a way for protecting the human health and the environment, but also an opportunity for the future reuse of materials and, then, for the enhancement of the circular economy" (European Environmental Bureau, 2017). While there are overlaps between the approaches of green chemistry and circular economy (Linder, 2017; Loste et al., 2020; Silvestri et al., 2021), green chemistry explicitly addresses human health, which is typically outside the scope of circular economy debates (Chen et al., 2020). Consequently, Murray et al. (2017) suggest incorporating "human well-being" into circular economy's definition (p. 377). However, the circular economy approach focuses primarily on economic factors (Inigo and Blok, 2019). Even though both green chemistry and circular economy aim to promote sustainable development, uncertainty and unexpected consequences can arise along research and innovation processes (Inigo and Blok, 2019). Therefore, research and innovation activities should be conducted responsibly, with future-focused consideration for ethical, social, political, legal and economic aspects, to ensure meaningful contributions towards the SDGs.

2.2. *Responsible research and innovation*

RRI represents a holistic approach to scientific and technological development that integrates societal values, ethical considerations, and the needs of diverse stakeholders throughout research and innovation processes (Owen et al., 2013; Stilgoe et al., 2013; von Schomberg, 2012). It is defined as "a transparent, interactive process by which societal actors and innovators become mutually responsive to each other with a view to the (ethical) acceptability, sustainability and societal desirability of the innovation process and its marketable products […]" (von Schomberg, 2012, p. 50). Four principles provide guidance for RRI: (1) *inclusion* emphasises the active involvement of diverse stakeholders throughout the research and innovation process to democratise decision-making and enhance legitimacy, (2) *anticipation* involves proactively identifying and addressing potential implications and uncertainties of research and innovation to minimize adverse outcomes and maximise positive ones, (3) *reflexivity* refers to the ongoing critical examination and evaluation of the underlying values, assumptions, and impacts of research and innovation to ensure alignment with societal values and ethical considerations, (4) *responsiveness* involves adapting R&D activities in response to feedback, emerging issues, uncovered uncertainties and evolving societal needs to ensure research and innovation remain accountable and socially beneficial (Owen et al., 2013; Stilgoe et al., 2013).

The RRI approach was used to guard the technological development in a number of fields such as nanotechnology, biotechnology, genetic engineering, digital technology including information and communication technology (Thapa et al., 2019; Timmermans, 2017), to mention but a few. While some scholars see the value of connecting green chemistry and RRI (Mehlich, 2018, 2023), a systematic literature search indicated that there are no examples, to the best of the authors' knowledge, of how RRI principles could be put into green chemistry practice (see Appendix A).

2.3. *Towards responsible green chemistry*

2.3.1. *Embedding RRI principles into green chemistry*

The understanding of responsible green chemistry is very limited with a notable contribution from Mehlich (2023) who argues that integrating RRI into green chemistry would enable chemists to "represent societal interests and environmental needs in one's daily practice" (p. 15). As green chemistry and circular economy are intertwined, some lessons can be learned from studies on RRI for circular economy (see Appendix A). These insights are discussed next.

Following the principle of *inclusion,* engaging different stakeholder groups is important to make sure that societal values, needs, and a wide range of perspectives are considered that helps to achieve socially desirable and acceptable outcomes as results of research and innovation processes (Stahl et al., 2014). In order to involve a diverse set of stakeholders, groups from industry, politics and society must be included (Purvis et al., 2023). Additionally, when involving stakeholders, it is important to ensure that both those directly affected along the value chain (e.g., suppliers, producers, users) and those who could be impacted by the outcomes (e.g., public, local communities) are heard (Purvis et al., 2023). Especially in the context of green chemistry, involving stakeholders might provide a 'just transition' "where the needs and rights of all stakeholders are taken into account" (Purvis et al., 2023, p. 2). Past studies in the context of circular economy practice argue that inclusion can be enabled by workshops (Castilla-Polo and Sánchez-Hernández, 2022), debates (Castilla-Polo and Sánchez-Hernández, 2022), and training for the public (Castilla-Polo and Sánchez-Hernández, 2022) as well as through inter- and transdisciplinary collaborations, for instance, with social sciences and humanities (Parada et al., 2022). Mutual learning can be also achieved through co-innovation (Castilla-Polo and Sánchez-Hernández, 2022), open innovation (Castilla-Polo and Sánchez-Hernández, 2022; Purvis et al., 2023), and user-centred designs (Castilla-Polo and Sánchez-Hernández, 2022; Purvis et al., 2023). Additional activities such as consensus conferences, citizens' juries, focus groups, science shops, deliberative mapping, and laypeople being members of expert bodies also enable inclusion of stakeholders in R&D activities (Purvis et al., 2023). However, whether the methods can be transferred to the field of green chemistry remains uncertain due to the lack of studies that attempt to integrate the principle of inclusion into green chemistry practice.

R&D activities that embrace the principle of *anticipation* are characterised by considerations for impacts and uncertainties (Owen et al., 2013; Stilgoe et al., 2013). Especially in the field of green chemistry anticipating intended and unintended impacts can help to raise "awareness of some of the upcoming issues" (Inigo and Blok, 2019, p. 285) and address potential tensions (Parada et al., 2022). In the practice of circular economy, anticipating potential impacts is performed by technology foresight (Inigo and Blok, 2019; Purvis et al., 2023), technology assessment (Purvis et al., 2023), 'safe by design' (Parada et al., 2022), 'value-driven design' (Parada et al., 2022), co-design (Parada et al., 2022), surveys (Castilla-Polo and Sánchez-Hernández, 2022), horizon scanning (Purvis et al., 2023), scenario building (Purvis et al., 2023), vision assessment (Purvis et al., 2023), and (social) life cycle assessment (Purvis et al., 2023). The use of these methods in early stages of research and innovation activities helps to "reflect [on] possible unintended side effects to prevent worsening the situation" (Schneider et al., 2021, p. 1090) and addresses potential consequences even in the face of uncertainty (Inigo and Blok, 2019). Particularly when potential applications of research and innovation are envisioned, RRI – including anticipation – should be integrated from the outset and embedded at early stages, rather than being added later or incorporated retrospectively (Owen et al., 2013). However, uncertainty remains, even if anticipatory activities are undertaken (Purvis et al., 2023). Anticipation in the early stages of research and innovation can be constrained by resources limitations, such as time and costs, as well as by the lack of supportive policies and tools, as observed in business contexts where RRI has been attempted to implement (Stahl et al., 2019). Furthermore, the anticipation methods might need to be customised in order to include indicators that are relevant to the SDGs (e.g., integrating SDGs into life cycle assessment methods, see Cordella et al. (2023)). The applicability of anticipatory methods to green chemistry is not yet established, given the lack of understanding on implementing the principle of anticipation in the field of green chemistry.

The principle of *reflexivity* can ensure the alignment with societal values and ethical considerations throughout the entire research and innovation process. In the context of green chemistry, constantly evaluating whether one is on the right track is particularly important, as technological developments and societal needs can change rapidly. Insights from past circular economy research suggest that the principle of reflexivity can be put into practice through multi-disciplinary collaboration (e.g., with social scientists and ethicists) and training (Purvis et al., 2023), codes of conduct (Castilla-Polo and Sánchez-Hernández, 2022; Inigo and Blok, 2019; Purvis et al., 2023), best practice guidelines (Castilla-Polo and Sánchez-Hernández, 2022), moratoria (Inigo and Blok, 2019; Purvis et al., 2023), and reflecting on roles and responsibilities (Purvis et al., 2023). However, it is still unclear whether the methods can be applied to the field of green chemistry, as there are no studies investigating how the principle of reflexivity can be integrated into green chemistry practice.

Last but not least, applying the *responsiveness* principle is of high importance because it combines the RRI principles by responding to the insights and feedback provided by the other principles. This is particularly important in the context of green chemistry, as new insights can lead to necessary changes in direction and adaptations to new, evolving societal needs. In recent circular economy research, this means responding to the insights that emerge when researchers interact with numerous stakeholders, are anticipative and reflective (Purvis et al., 2023). The flexibility to change direction based on constant feedback can be achieved when researchers pursue 'strategic niche management', 'value-driven design', 'sustainable design', moratoria, stage gates, alternative intellectual property regimes, incremental scaling-up, adaptive risk management, living labs, and social experimentation, as well as flexible and adaptive design (Purvis et al., 2023). Ensuring a high level of transparency in R&D projects can be supported by defining grand challenges and thematic research programmes (Purvis et al., 2023), regulation and standards (Purvis et al., 2023), open access (Purvis et al., 2023), and other transparency mechanisms (Castilla-Polo and Sánchez-Hernández, 2022; Purvis et al., 2023). Due to the absence of studies investigating the integration of the principle of responsiveness into green chemistry practice, it remains uncertain if the methods can be adapted to this field.

In summary, it is unclear whether the methods within recent circular economy research can be directly applied to the context of green chemistry. There is a lack of understanding on how to integrate the RRI principles into green chemistry practice.

2.3.2. *Tools for embedding RRI principles into planning R&D*

We have shown above that there are some but limited insights into how to make green chemistry research and innovation processes more responsible. The problem is however not unique to this scientific field. In line with Shelley-Egan et al. (2018), it is a key challenge to figure out how to embed RRI into the routines of professional researchers and "more importantly, how can RRI activities be embedded so that they are valued by the research organisation itself as being part of each individual researcher's core activities and evaluated as such within research institutions, rather than (at best) interesting side projects or (at worst) distractions from the core activity of research." (Shelley-Egan et al., 2018, p. 1740).

Particularly promising are approaches that allow to embed the RRI philosophy in the early stages of research and innovation processes as at that point in time it is still possible to have significant influence on the direction and outcomes of R&D endeavours (Owen and Goldberg, 2010; Shelley-Egan et al., 2018). Among such approaches are RRI roadmaps. Roadmaps generally serve as "a strategic plan that defines a goal or desired outcomes, and includes the major steps or milestones needed to reach it." (Porcari et al., 2019, p. 5). Over 20 years, different schools in roadmapping have evolved consisting of different "(a) research orientation, whether it be solution- or theory-oriented; (b) the research methods and data sources being used; and (c) the nature of contributions that each school seeks to achieve." (Park et al., 2020, p. 10). Similarly, we see the potential in combining roadmapping concepts from different schools and developing hybrid approaches, rather than viewing them as independent entities (Park et al., 2020).

However, there are only few examples in the RRI literature where the roadmapping method is used to integrate RRI principles (Neuberger et al., 2024; Porcari et al., 2019) (see Appendix B for a literature review). Previous studies show and suggest that responsible roadmapping is a useful method for (a) responsible product development across different industry sectors (Porcari et al., 2019), (b) developing and implementing measures to facilitate the transition to digitalisation in pilot regions (Neuberger et al., 2024), and (c) developing RRI practices to leverage synergies among research projects to enhance the impact and relevance of the research (Aicardi et al., 2018). However, by focusing on long-term strategies for companies (Porcari et al., 2019), there is a missed opportunity to provide guidance for planning R&D activities from the early beginning and beyond the scope of industrial context. Furthermore, by using "RRI-oriented roadmapping" as a "co-creation activity" (Neuberger et al., 2024, p. 10), the emphasis lies on engaging diverse stakeholder groups, rather than on ensuring a broad range of responsible actions – including anticipation, reflexivity, and responsiveness – throughout the entire process. Additionally, it could be assumed that developing RRI roadmaps as part of projects with EU funding (e.g., Aicardi et al., 2018; Neuberger et al., 2024; Porcari et al., 2019) entails different circumstances than those faced by researchers when they are in the early stages of planning their R&D endeavours. Therefore, based on the lack of literature, the aim of this study is to test if a roadmapping method can be adapted to embed the principles of RRI in research and innovation activities in green chemistry.

3. Methodology

To explore if and how the roadmapping method can help to develop broad research and innovation agendas that address technical, environmental as well as social, ethical, economic and political aspects in the complex transformations of industrial sectors, we propose a responsible roadmapping method and analyse the use of the method in three different cases within the field of green chemistry.

3.1. *Responsible roadmapping method*

There is very little overlap in the debates on RRI and roadmapping (Aicardi et al., 2018; Neuberger et al., 2024; Porcari et al., 2019) which is surprising given that roadmaps are tools for creating desired future outcomes. Taking inspiration from Porcari et al. (2019), we develop a responsible roadmapping method for integrating RRI principles into research and innovation activities. The responsible roadmap consists of seven elements such as the *objectives* (positive impacts researchers want to make relating to the SDGs), potential *challenges* and *barriers* that could be encountered that hinder achieving the envisioned research objective as well as potential *risks* (unwanted/unfavourable outcomes that are possible/probable). Additionally, the *RRI activities* define actions that could be done to overcome the challenges and barriers and to prevent and mitigate the risks. The *R&D steps* indicate activities that will be needed to achieve the research objective and bring it to use based on a *time* dimension.

Applying the responsible roadmapping method follows the same procedure for each research project: First, a preliminary version of the responsible roadmap was developed by the research team. During a 2-h online meeting, two moderators (first and second author) asked step-by-step questions to aid the development of the responsible roadmap. Second, to expand the preliminary version, a 4-h 'responsible roadmap workshop' was conducted online with 21 participants from five different research disciplines. Participants identified additional challenges, barriers, and risks and integrated further RRI activities through brainstorming and group discussions.

The RRI principles are embedded during the responsible roadmapping method in different ways. The participation of researchers from different disciplines in the 'responsible roadmap workshop' ensures the involvement of a variety of perspectives and fosters inter- and transdisciplinary collaborations. This approach promotes the principle of *inclusion* by integrating diverse viewpoints. Considering challenges, barriers, and risks during the planning stages of R&D activities allow for the incorporation of the principles of *anticipation* and *reflexivity*. The responsible roadmaps result in action plans that already include RRI activities addressing potential challenges, barriers, and risks. These plans allow for continuous adaptability as needed, aligning with the principle of *responsiveness*.

Thus, applying the responsible roadmapping method should enable researchers to incorporate RRI principles into the planning of their R&D activities and to shape their research action plans more responsibly by going beyond technological and environmental considerations and human health issues to include socio-ethical, policy, and economic considerations.

3.2. *Case selection and analysis*

We analysed the use of the responsible roadmapping method in three cases. In the selection of cases, we sought the heterogeneity of potential industrial application of the green chemistry processes and products, varying levels of interdisciplinarity among research teams, and varying Technology Readiness Levels (European Commission et al., 2017). The research projects had to be in the early planning stage. Based on these criteria, we selected three research projects in the field of green chemistry aiming to contribute to the circular economy agenda.

All research teams were in the process of planning their next steps to develop technological solutions for different industrial problems. Their joint aim is to shift traditional production practices towards more sustainable and safer ones and increasing the circular economy. However, the cases differ in the degree to which the teams are interdisciplinary and in the Technology Readiness Level of their innovation (ranging from one to four). All research teams are aware of many technological (e.g., material durability, toxicity of materials), environmental (e.g., energy consumption, unintended environmental impacts), and human health (e.g., potential health risks) challenges that need to be overcome in order to achieve their envisioned outcomes. They also find it important to consider potential socio-ethical (e.g., stakeholder acceptance, risk aversion of customers), policy (e.g., regulations and standards), and economic considerations (e.g., financial viability, competitiveness compared to other innovations). Hence, the three research projects represent promising cases that could benefit from embedding RRI principles in their R&D activities in green chemistry contributing to the circular economy.

The analysis of the cases involves two approaches: First, examining the roadmaps to identify challenges, barriers, risks, and RRI activities related to the 12 principles of green chemistry (technological, environmental, and human health considerations) and those that extend beyond them (socio-ethical, policy, and economic considerations). Second, assessing the roadmap elements introduced during the 'responsible roadmap workshop' to evaluate the significance of this collaborative activity (see Appendix C).

4. Results

4.1. Case 1: Aquapur

4.1.1. Case introduction

Water is essential for life and ensuring a clean and safe water supply is crucial. Wastewater treatment processes include primary treatment for removing large solids, secondary treatment for degrading organic matter biologically, and tertiary treatment for advanced water purification. However, conventional wastewater treatment processes cannot fully remove trace organic contaminants such as pharmaceuticals, pesticides, or flame retardants, posing a risk to aquatic ecosystems and drinking water resources (Eggen et al., 2014; Luo et al., 2014; Schwarzenbach et al., 2006). To enhance the removal of organic contaminants from wastewater, additional treatment steps are needed (Eggen et al., 2014). As alternative to activated carbon, which is commonly used in water treatment, sustainable bio-based materials bear promise to remove trace organic contaminants from water.

4.1.2. Responsible roadmap

The aim of the Aquapur research project is to develop adsorber materials to reduce and remove organic contaminants in water based on bio-polymers recycled from industrial food and paper industry waste. Positive impacts on the environment will be achieved through the use of recycled bio-based materials, the reuse of waste materials and by keeping waste materials in a cycle for beneficial use (e.g., for water treatment) (see Fig. 1). Furthermore, the elimination of trace organic contaminants from water will help to reduce ecological and human health risks in the long term and contribute to meeting several SDGs.

The research team is aware of several challenges, barriers, and risks that might arise during their course of R&D. In order to address these potential issues, different (responsible) research activities are planned: *Technological* considerations such as the stability and longevity of the water treatment materials as well as the effectiveness for contaminant removal will be addressed through conducting stability tests. The possibility of recovering organic chemicals as a 'recycling' option is taken into account as further *environmental* considerations. Toxicity tests at different points of time along the R&D process and a careful selection and close engagement with waste material suppliers will help to reduce safety and *human health* concerns such as potential toxicity and risks of the novel materials.

The researchers also identified considerations that go beyond the 12 principles of green chemistry by taking socio-ethical, policy, and economic considerations into account. Considering *socio-ethical* dimensions, the question of acceptance of future users of the novel materials will be tackled by engaging with industry, wastewater treatment plant operators, and cities. *Policy* considerations like the legislation of novel materials will be addressed by conducting an innovation system analysis and identifying and collaborating with regulatory experts. *Economic* considerations meaning financial viability and competitiveness compared to other water treatment materials and processes will be investigated by assessing the costs already at early stages of their R&D process.

In particular, the interdisciplinary discourse during the 'responsible roadmap workshop' enabled the researchers to go beyond the 12 principles of green chemistry and to make additional considerations that they were not initially aware of at the beginning of the responsible roadmapping process (see Appendix C).

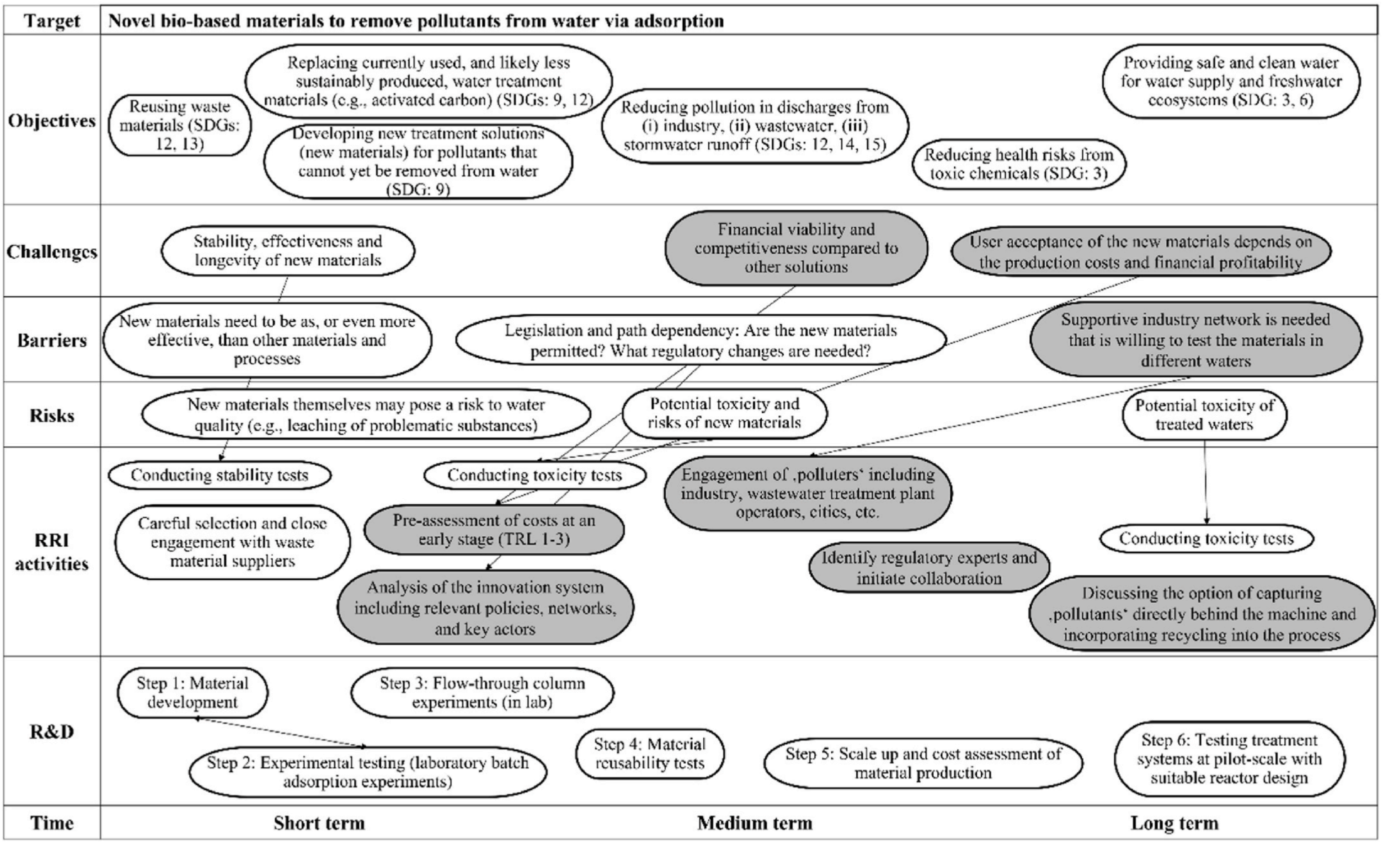

Fig. 1. Responsible roadmap of Aquapur.
Note. The colour grey indicates elements that go beyond the 12 principles of green chemistry. Arrows indicate relationships between the elements.

4.2. *Case 2: Liqchlor*

4.2.1. *Case introduction*

Chlorine is used in many different fields of application and is the basis for a number of industrial compounds (Lin et al., 2017; Winder, 2001). Nevertheless, chlorine poses risks due to its high reactivity and toxicity (Winder, 2001). Traditional storage and transportation methods also pose a threat (Hearn et al., 2013). Furthermore, in 2018, chlorine production through chlor-alkali electrolysis accounted for 4.25 % of total industrial electricity consumption in Germany (Roh et al., 2019). In order to enable safer and more sustainable use of chlorine, the method of chlorine storage should be considered further. Decentralised and mobile chlorine storage could reduce hazards and ensure a more sustainable use of chlorine.

4.2.2. *Responsible roadmap*

The research project Liqchlor aims to develop a demonstrator for decentralised chlorine storage using ionic liquids with potential applications in water purification. Developing a demonstrator for decentralised chlorine storage might bring important improvements of traditional chlorine usage and storage: Improving the safety of chlorine storage and facilitating a more sustainable chlorine production by enabling the use of renewable energy (see Fig. 2). In the long run, there is the potential of applying stored chlorine in water purification in low- and middle-income countries and contributing to various SDGs.

The research team recognises several challenges, barriers, and risks that could emerge during their R&D process. To address these potential issues, they plan various (responsible) research activities: Engaging and networking with partners to decide on applications will address the identified *technological* considerations that the identification and selection of partners for first (and different) applications need to be prioritised. *Environmental* impacts could be caused by the transport of stored chlorine, the energy consumption during releasing the stored chlorine, and disposal of potential waste. Therefore, partners will be selected for waste disposal, a deposit system will be considered and collaboration with the German government environmental agency will be initiated. Also, general *human health* concerns, including safety and security, such as toxicity of the materials will be addressed by engaging with partners assessing the safety and toxicity of the materials. Furthermore, there is the possibility that the waste may be disposed with unintended contamination that will be handled by a careful selection of the partners for disposal.

The researchers' consideration also broadens the scope of the green chemistry framework by taken into account *socio-ethical* considerations including the acceptance of potential users and society as well as the advertisement issues of chlorine as it might be a controversial topic. These issues will be addressed by involving social sciences investigating controversies on chlorine usage and demonstrating successful applications in cooperation with the industry. *Policy* considerations have not arisen during the planning of their R&D activities. *Economic* considerations including the financial viability and competitiveness compared to other innovative solutions will be addressed by linking technical and cost assessments.

Notably, the interdisciplinary discussions held during the 'responsible roadmap workshop' allowed the researchers to extend beyond the 12 principles of green chemistry and incorporate these additional considerations that were not recognised at the start of the responsible roadmapping process (see Appendix C).

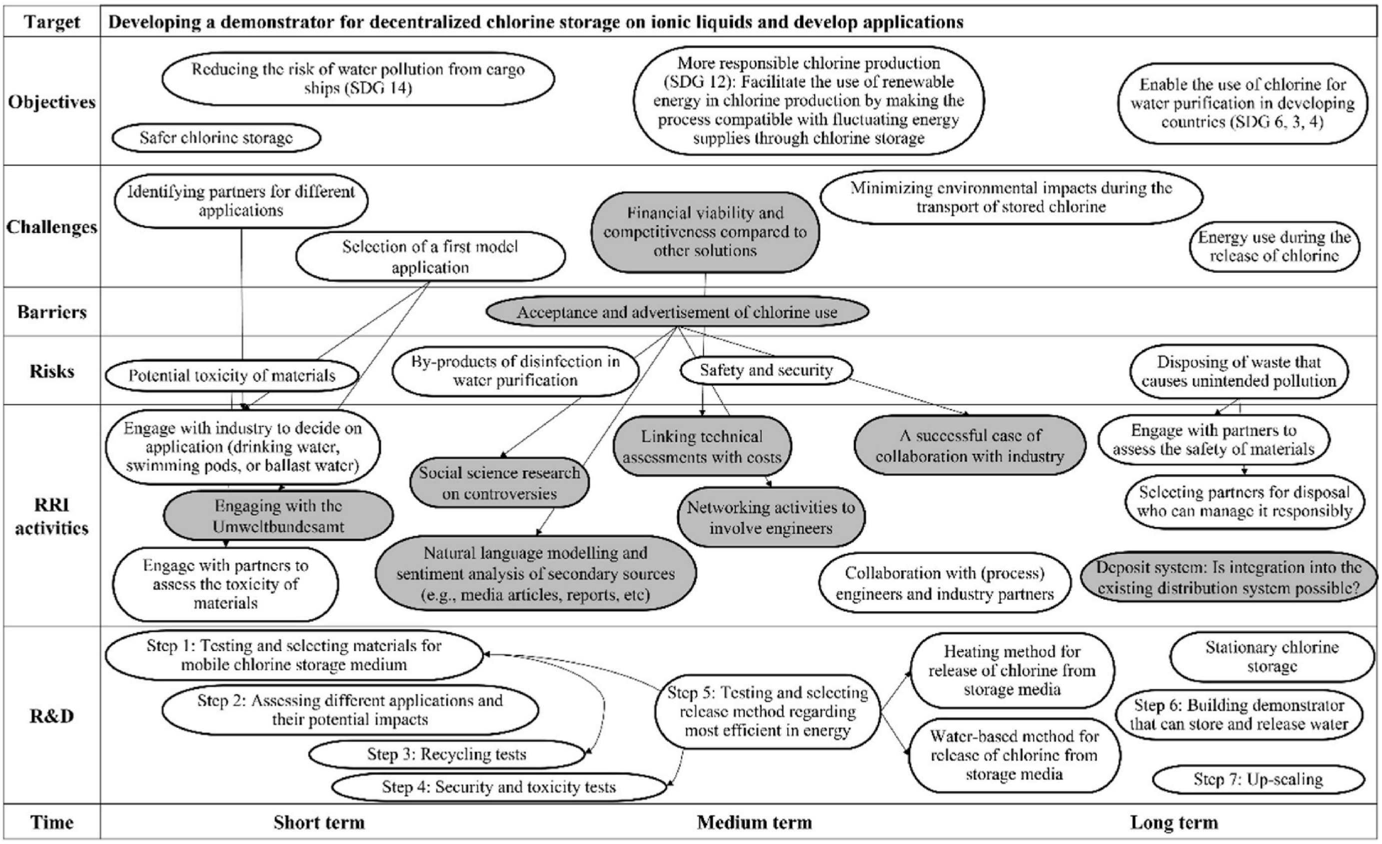

Fig. 2. Responsible roadmap of Liqchlor.
Note. The colour grey indicates elements that go beyond the 12 principles of green chemistry. Arrows indicate relationships between the elements, Umweltbundesamt = German government environmental agency.

4.3. Case 3: Binding materials

4.3.1. Case introduction

Construction and demolition by-products are one of the largest waste streams in the European Union. The construction and demolition industries were responsible for 37.5 % of the total waste generated from all industrial sectors in the European Union (Eurostat, 2024). Construction and demolition by-products consist of a wide range of raw materials including soil, concrete, sand, bricks, tiles, treated and untreated wood, roofing shingles, dry wall, and glass that can be returned to the material cycle after physical processes (Li et al., 2013). However, in many cases the quality of recovered construction and demolition by-products is less than similar materials obtained from nature or related industries. This issue eclipses the sustainability of recovery and returning construction and demolition waste in the material cycle. The main reason for this challenge is ignoring chemical treatments in recycling construction and demolition by-products.

4.3.2. Responsible roadmap

The aim of the binding materials research endeavour is to recycle construction and demolition by-products into basic materials through chemical treatments and, if necessary, using additive manufacturing, commonly known as 3-D printing. Potential applications include construction road and composite industries resulting in more sustainable solutions than traditional processes and a reduction of CO_2 emissions. Recycling construction and demolition by-products would lead to no need of purchasing new materials and a (new) use case for these materials would be created by recycling and transferring the by-products into useful materials (see Fig. 3). Furthermore, it might increase the processability and improve the quality of construction and demolition by-products as well as a more resource-efficient material usage by 3-D printing as it is already demonstrated (e.g., by Amir (2013)). Achieving their envisioned research objective will contribute to several SDGs.

However, the research team is aware of multiple challenges, barriers and risks that could arise during their course of R&D. In order to address these potential issues, different (responsible) research activities are planned: To achieve the *technological* necessary fresh state and long-term mechanical and durability properties, a real-world demonstrator will be developed and alternative applications considered. Planned activities concerning the *environmental* properties that need to be achieved and potential unintended environmental impacts are still unresearched. Potential unintended *human health* impacts will be considered and investigated by conducting assessments to evaluate potential unintended health risks and the toxicity of materials.

Furthermore, the researchers go beyond the green chemistry approach by considering *socio-ethical* dimensions including the acceptance of stakeholders and customers (e.g., road authorities, construction work companies) that will be addressed by preparing an early-stage demonstration of application in a real-world environment, engaging road authorities and quantifying externalities of the innovation in comparison with the traditional application. Furthermore, through the quantification of externalities of their innovation and conventional application, the conflict will be addressed that the use of biodiesel is utilised for the production of the binding materials instead of food purposes. Furthermore, there might arise commercial problems if the price for CO_2 emission certificates does not increase as expected. Therefore, *policy* considerations will involve discussing the problem of overregulation and that political decisions need to provide long-term security. *Economic* considerations include financial viability and competitiveness compared to other innovations and industries (e.g., oil industry) as well as that the materials might not be available in the

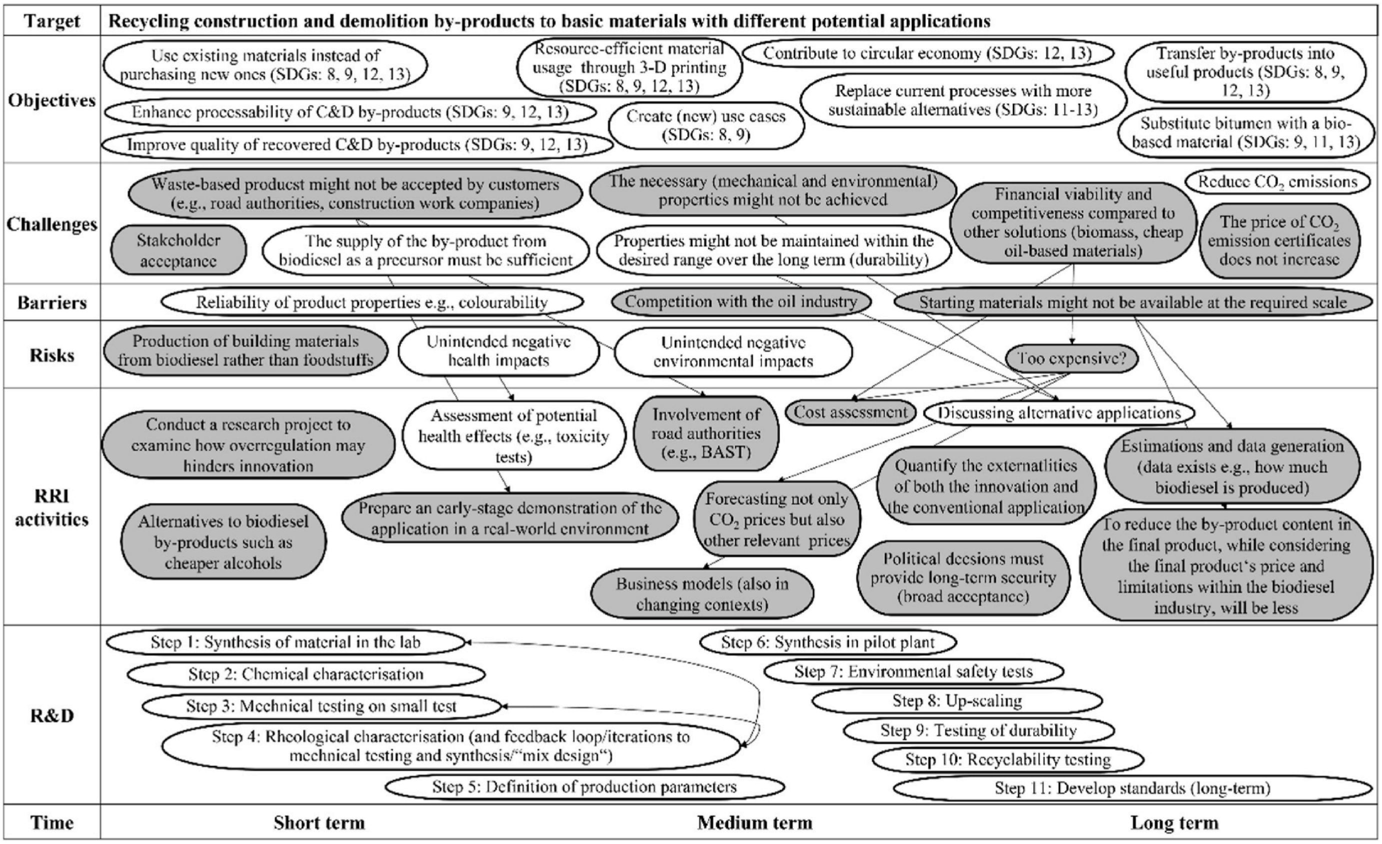

Fig. 3. Responsible roadmap of Binding materials.
Note. The colour grey indicates elements that go beyond the 12 principles of green chemistry. Arrows indicate relationships between the elements, BASt = German Federal Highway Research Institute.

required scale at the beginning. That will be addressed by taking into account cheaper alternatives for the required by-products, conducting cost assessments considering CO_2 prices, and developing possible business models.

Especially, the interdisciplinary discourse during the ‘responsible roadmap workshop’ supports the researchers to go beyond the 12 principles of green chemistry and to detect further considerations that are not primarily identified by themselves (see Appendix C).

5. Discussion

The aim of this study was to bring together the green chemistry and RRI and to investigate *how the principles of RRI can be embedded in the development of green chemistry products and processes* with the view to help green chemistry to contribute towards the transition towards sustainable production modes and the achievement of the SDGs. We proposed and tested a responsible roadmapping method for integrating social, ethical, political, legal and economic aspects into the development of green chemistry products and processes. The method was applied in three research projects originating in the field of green chemistry and aiming to contribute to the circular economy agenda and numerous SDGs. During the responsible roadmapping process the research teams elaborated their objectives, identified different challenges, barriers, and risks and developed plans for addressing them with several (responsible) activities.

The study finds that responsible roadmapping method has been useful in helping researchers to consider ethical, social, political, legal and economic aspects related to the green chemistry products and processes that the researchers aspired to develop. The method allowed the development of three distinct action plans for trans- and interdisciplinary research and innovation, aiming to contribute to the circular economy and various SDGs. This roadmapping method helps to develop action plans that adhere to the principles of RRI, as demonstrated in previous studies in other contexts (e.g., Neuberger et al., 2024; Porcari et al., 2019). The planned activities align with the 12 principles of green chemistry (American Chemical Society, 2024a) but also extend beyond them by considering broader socio-ethical, policy, and economic aspects. Especially the interdisciplinary approach used during the workshop gave the research teams the opportunity to go beyond the scope of the green chemistry principles and take a wider range of considerations into account. Interdisciplinary collaboration mediated by the roadmapping process proved valuable in integrating multiple perspectives and embedding socio-ethical dimensions into R&D (Flipse et al., 2014).

The study’s contribution to the literature is threefold: First, it addresses the gap in the field of green chemistry going beyond the in-depth considerations of environmental and human health issues and pay more attention to socio-ethical, policy, and economic issues (Falcone and Hiete, 2019; Mehlich, 2023). Second, the study contributes to the RRI literature by illustrating how RRI principles can be embedded into the planning of R&D activities in green chemistry. While previous studies have only conceptually attempted to bridge these fields (Mehlich, 2023), our study is the first attempt to provide practical insights on how to achieve this integration. Third, it demonstrates that the responsible roadmapping method can be adapted to integrate RRI principles within contexts beyond industrial applications (Porcari et al., 2019) and regional digital transitions (Neuberger et al., 2024).

The study has practical implications for chemistry research and innovation activities. The responsible roadmapping method could be used in both public and private sectors to identify the social, ethical, political, legal and economic aspects related to the new chemical products and processes and to plan how to address them during the R&D activities. The method is considered robust enough to be also applicable in other technological fields, with potential modifications needed. Furthermore, it is recommended to incorporate the responsible roadmapping method into the higher education curricula for natural science students in order to enhance their skills for steering their future research and innovation activities towards the SDGs (see Gerrits et al., 2022; Tassone et al., 2018). The implications for science policy can also be drawn from this study. Funders interested in supporting responsible, trans- and interdisciplinary research could require a submission of responsible roadmaps as part of grant applications to encourage responsible approach to research and innovation from the outset (Owen and Goldberg, 2010).

However, some limitations of this study need to be acknowledged. First, we tested the responsible roadmapping method on a limited number of non-representative cases, which weakens its generalisability, in particular to non-technical research projects. Although we aimed for diversity in industrial application, interdisciplinarity among research teams, and varying Technology Readiness Levels, future research should apply the responsible roadmapping method to additional research projects within and beyond green chemistry to verify its generalisability. Second, our study focused on incorporating RRI principles in R&D plans. However, it could not examine if the developed action plans could be translated into successful research project applications and realised in practice. Future research should either accompany the research teams during the fund raising and implementation phases or conduct retrospective interviews.

6. Conclusion

In conclusion, chemical products and processes could play a key role in enabling transition to more sustainable production modes, supporting the circular economy, and addressing the SDGs. Green chemistry aims to reduce and eliminate hazardous substances while promoting environmental and human health, resource preservation, and economic viability. This study bridges an important gap by suggesting how to integrate Responsible Research and Innovation principles into green chemistry practices through the use of responsible roadmapping method. Applying this method to three research projects focusing on sustainable and safer production practices, led to distinct action plans for trans- and interdisciplinary research and responsible innovation. Interdisciplinary roadmapping process expanded the scope of these plans, incorporating relevant social, ethical, political, legal and/or economic aspects. The study demonstrates that by using responsible roadmaps researchers can be empowered to take responsibility for co-creating sustainable futures through their R&D activities, to plan how to enhance the desirable impacts of their research and innovation while minimising risks and negative impacts.

Declaration of generative AI and AI-assisted technologies in the writing process

During the preparation of this work the authors used ChatGPT-3.5 in order to improve readability and language of the work. After using this tool, the authors reviewed and edited the content as needed and take full responsibility for the content of the published article.

Funding sources

We gratefully acknowledge financial support from the Einstein Research Unit “Climate and Water under Change” from the Einstein Foundation Berlin and Berlin University Alliance (Grant ERU-2020-609).

CRediT authorship contribution statement

Madita Amoneit: Writing – review & editing, Writing – original draft, Visualization, Methodology, Investigation, Formal analysis, Conceptualization. **Dagmara Weckowska:** Writing – review & editing, Supervision, Project administration, Methodology, Conceptualization. **Stephanie Spahr:** Writing – review & editing. **Olaf Wagner:** Writing – review & editing. **Mohsen Adeli:** Writing – review & editing. **Inka Mai:**

Writing – review & editing. **Rainer Haag:** Writing – review & editing, Funding acquisition.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgement

We would like to thank Alejandro Lorente, Dietmar Stephan, Patrick Voβnacker, and Sebastian Hasenstab-Riedel (in addition to the co-authors) for providing us with their research projects as exploratory cases, for their co-operation and effort in developing the roadmaps. We would like to thank all workshop participants who contributed to the workshop discussions. We would also like to acknowledge the Open Access Funding provided by Freie Universität Berlin.

Appendix A

To identify relevant literature to investigate RRI activities in green chemistry and circular economy research and innovation, a systematic literature review was conducted following the Preferred Reporting Items for Systematic reviews and Meta-Analyses (PRISMA) statement (Page et al., 2021; Rethlefsen et al., 2021) (see Figure A1). The literature search was conducted in the ‘Web of Science’ database from February to May 2024. The search was limited to publications in the English language and published between 2013 and 2024, given that the RRI principles have been first introduced by Owen et al. (2013) and Stilgoe et al. (2013). Reference lists of included articles were manually screened to identify additional studies (forward and backward search). Duplicates were removed manually. Two consecutive searches were carried out, specialising in the subjects of green chemistry and circular economy. A total of 820 articles were retrieved from the database (duplications already excluded). The following exclusion criteria applied in the screening process: (1) only journals with an impact factor equal to or higher than ten are considered (Clarivate, 2023). With the exception of the *Journal of Responsible Innovation* as a highly relevant journal in the scientific community that is of interest for the investigation and the publication from Parada et al. (2022). (2) RRI has to be understood according to Owen et al. (2013) and Stilgoe et al. (2013). (3) Green chemistry and circular economy have to be understood according to substances Anastas and Williamson (1996) and MacArthur (2013) respectively. The search strings that were successively applied can be found in Table A1. The four articles identified are Castilla-Polo and Sánchez-Hernández (2022), Inigo and Blok (2019), Parada et al. (2022), and Purvis et al. (2023).

Table A1
Applied search strings for the systematic literature review in four rounds

	Green chemistry	Circular economy
First round	“Responsible Research and Innovation” OR “RRI” OR “responsible research*” OR “responsible innovation*” AND “green chemistry”[1]	“Responsible Research and Innovation” OR “RRI” OR “responsible research*” OR “responsible innovation*” AND “behaviour*” OR “behavior*” OR “practice*” OR “action*” OR “activit*” AND “circular economy” OR “circularity”
Second round	“Responsible Research and Innovation” OR “RRI” OR “responsible research*” OR “responsible innovation*” OR “social innovation” OR “sustainable innovation” OR “ethical innovation” AND “behaviour*” OR “behavior*” OR “practice*” OR “action*” OR “activit*” AND “green chemistry”	“Responsible Research and Innovation” OR “RRI” OR “responsible research*” OR “responsible innovation*” OR “social innovation” OR “sustainable innovation” OR “ethical innovation” AND “behaviour*” OR “behavior*” OR “practice*” OR “action*” OR “activit*” AND “circular economy” OR “circularity”
Third round	“inclusion” OR “inclusiveness” OR “inclusive” AND “behaviour*” OR “behavior*” OR “practice*” OR “action*” OR “activit*” AND “green chemistry”	“inclusion” OR “inclusiveness” OR “inclusive” AND “behaviour*” OR “behavior*” OR “practice*” OR “action*” OR “activit*” AND “circular economy” OR “circularity”
	“anticipation” OR “anticipative” AND “behaviour*” OR “behavior*” OR “practice*” OR “action*” OR “activit*” AND “green chemistry”	“anticipation” OR “anticipative” AND “behaviour*” OR “behavior*” OR “practice*” OR “action*” OR “activit*” AND “circular economy” OR “circularity”
	“reflexivity” OR “reflective” AND “behaviour*” OR “behavior*” OR “practice*” OR “action*” OR “activit*” AND “green chemistry”	“reflexivity” OR “reflective” AND “behaviour*” OR “behavior*” OR “practice*” OR “action*” OR “activit*” AND “circular economy” OR “circularity”
	“responsiveness” OR “responsive” AND “behaviour*” OR “behavior*” OR “practice*” OR “action*” OR “activit*” AND “green chemistry”	“responsiveness” OR “responsive” AND “behaviour*” OR “behavior*” OR “practice*” OR “action*” OR “activit*” AND “circular economy” OR “circularity”
Fourth round	“Responsible Research and Innovation” OR “RRI” OR “responsible research*” OR “responsible innovation*” In selected journals: *Business Strategy and the Environment, Journal of Business Research, Journal of Cleaner Production, Journal of Environmental Management, Journal of Industrial Ecology, Journal of Responsible Innovation, Resources Conservation and Recycling*	

[1] The inclusion of search strings such as behaviour, practices, and activities (as in the first round of circular economy) made no difference in the results, so the minimal principle was applied.

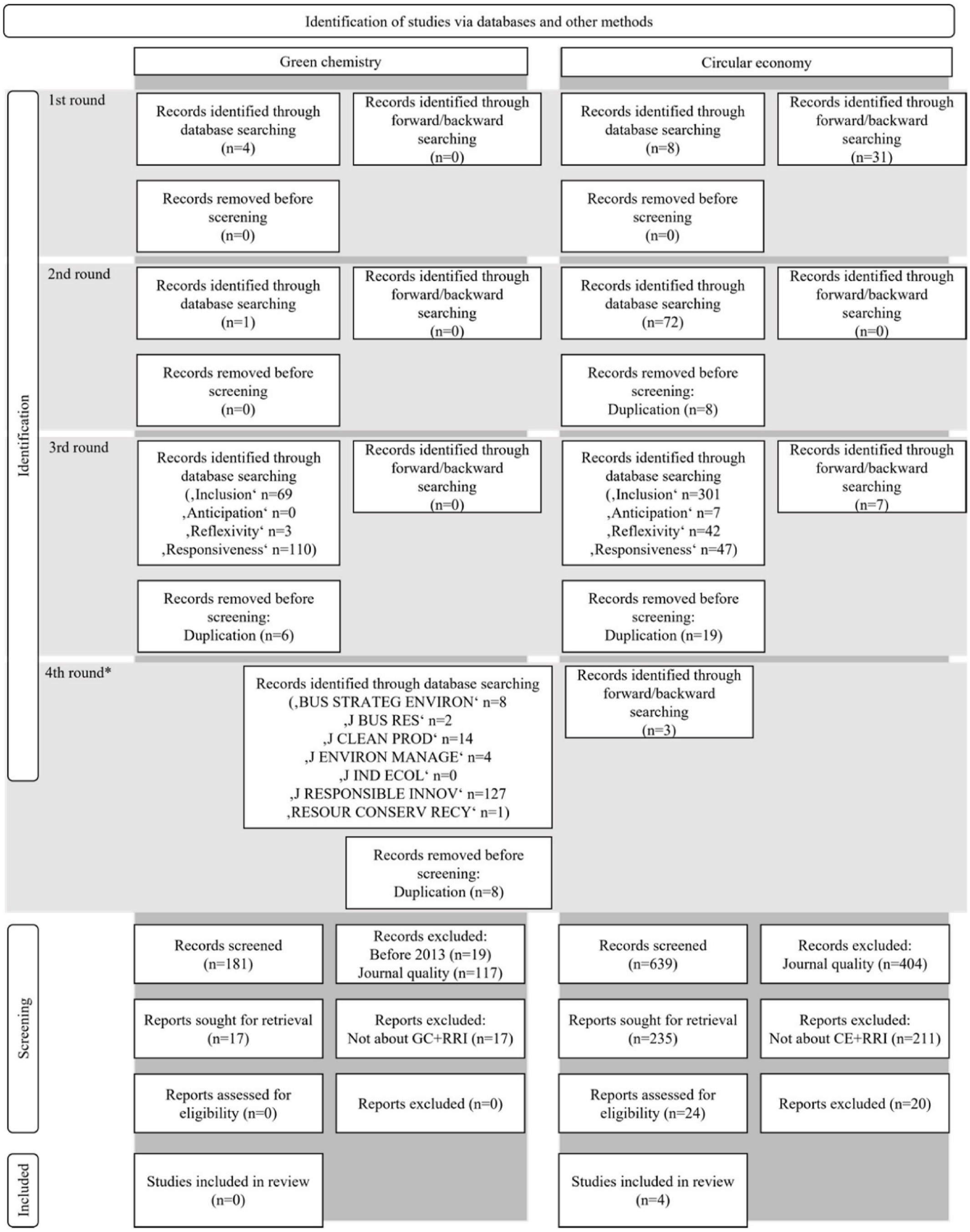

Fig. A1. Systematic literature review PRISMA flowchart. *Note.* GC = Green Chemistry, CE = Circular Economy.

Appendix B

Table B1
Search results of the literature review on RRI roadmaps

Search strings	Web of Science		Google Scholar	
	unspecific roadmap	responsible roadmap	unspecific roadmap	responsible roadmap
"(responsible) roadmap"	31,672	0	2,370,000	14
"(responsible) technological roadmap" OR "(responsible) technology roadmap"	1140	0	17,600	0
"(responsible) research roadmap"	393	0	34,800	0

(*continued on next page*)

Table B1 (*continued*)

Search strings	Web of Science		Google Scholar	
	unspecific roadmap	responsible roadmap	unspecific roadmap	responsible roadmap
“(responsible) strategic roadmap” OR “(responsible) strategy roadmap”	201	0	16,800	0
“(responsible) scientific roadmap” OR “(responsible) science roadmap”	52	0	3370	0
“(responsible) innovative roadmap” OR “(responsible) innovation roadmap”	44	0	3210	3
“(responsible) research and innovation roadmap”	2	0	646	3

Note. Only RRI literature that defines RRI according to the four key principles (inclusion, anticipation, reflexivity, and responsiveness), as outlined by Owen et al. (2013) and Stilgoe et al. (2013), was considered. The search strings were applied in all search fields. The term ‘responsible’ was only used for searches that lead to search results in the ‘responsible roadmap’ columns. The search was performed on September 20, 2024. The search results are not displayed here if (a) article were redundant, (b) were only citations instead of full articles, and (c) were not English-written articles. The use of ‘roadmapping’ instead of ‘roadmap’ was also considered in the search strings, but the use of ‘responsibility’ instead of ‘responsible’ made no difference in finding relevant search results, so they do not appear in the table. All results in the ‘responsible roadmap’ columns were checked for relevance by reading abstracts.

Appendix C

Table C1

Considerations taken into account by the research team *at the start* of the responsible roadmapping process and additional considerations identified *during* the responsible roadmapping process (both categorised as technological, environmental, human health, socio-ethical, policy, and economic).

Type of considerations	Case 1: Aquapur		Case 2: Liqchlor		Case 3: Binding materials	
	Challenges, barriers and risks	RRI activities	Challenges, barriers and risks	RRI activities	Challenges, barriers and risks	RRI activities
Technological	*At the start:* Stability, effectiveness and longevity of new materials (C) New materials need to be as or even more effective than other materials and processes (B) *During process:* /	*At the start:* Conducting stability tests *During process:* /	*At the start:* Identifying partners for different applications (C) *During process:* Selection of a first model application (C)	*At the start:* / *During process:* Successful case in collaboration with industry Networking activities to involve engineers Collaboration with (process) engineers and industry partners	*At the start:* Supply of the by-product from biodiesel as a precursor must be sufficient (C) Properties cannot be maintained in a long-term in the desired range (durability) (C) *During process:* Reliability of properties of products, e.g., colourability (B)	*At the start:* / *During process:* Discussing alternative applications
Environmental		*At the start:* / *During process:* Discussing the option of recollection of ‘pollutants’ directly behind a machine and addition of the application of ‘recycling’	*At the start:* Minimising the environmental impacts during transport of stored chlorine (C) Use of energy in release of chlorine (C) By-products of disinfection in water purification (R) *During process:* /	*At the start:* Selecting partner for disposal that can do it well *During process:* Engaging Umweltbundesamt Deposit system: Is an integration in existing distribution system possible?	*At the start:* Necessary (mechanical and environmental) properties might not be achieved (C) Reduce CO_2 emissions (C) Unintended negative environmental impact (R) *During process:* /	
Human health	*At the start:* Potential toxicity and risks of new materials (R) Potential toxicity of treated waters (R) *During process:* New materials themselves may pose a risk for water quality (e.g., leaching of problematic substances) (R)	*At the start:* Conducting toxicity tests (at the beginning and end) Careful selection and close engagement with waste material suppliers *During process:* /	*At the start:* Potential toxicity of materials (R) Safety and security (R) Disposing waste with unintended pollution (R) *During process:* /	*At the start:* Engage with partners to assess the toxicity of materials Engage with partners to assess the safety of materials Selecting partner for disposal that can do it well[1] *During process:* /	*At the start:* Unintended negative health impact (R) *During process:* /	*At the start:* / *During process:* Assessment of possible health effects (toxicity tests)
Socio-ethical	*At the start:* / *During the process:* The acceptance of the new materials by users is dependent on the production costs and financial profitability (C) Industry network	*At the start:* Engagement of ‘polluters’ (industry, wastewater treatment plant operators, cities, etc.) *During the process:* /	*At the start:* / *During the process:* Acceptance and advertisement of chlorine topic (B)	*At the start:* Engage with industry to decide on application (drinking water, swimming pods, or ballast water) *During the process:* Natural language modelling and sentiment analysis on secondary	*At the start:* Waste-based product might not accept by customers (road authorities, construction work companies) (C) Production of building materials (biodiesel) instead of foodstuff (R)	*At the start:* Involvement of road authorities (e.g., BASt) *During the process:* Prepare early-stage demonstration of application in a real-world environment Quantify externalities

(*continued on next page*)

Table C1 (*continued*)

Type of considerations	Case 1: Aquapur		Case 2: Liqchlor		Case 3: Binding materials	
	Challenges, barriers and risks	RRI activities	Challenges, barriers and risks	RRI activities	Challenges, barriers and risks	RRI activities
	willing to test materials in different waters (B)			sources (media articles, reports, etc.) Social science on controversies	*During the process:* Acceptance of stakeholders (C)	of the innovation and the conventional application
Policy	*At the start:* / *During the process:* Legislation and path dependency: Are the new materials allowed? How have regulations to be changed? (B)	*At the start:* / *During the process:* Innovation system analysis including analysis of relevant policies, networks and actors Address responsible actors in the municipalities and authorities Identify regulatory experts and initiate collaboration			*At the start:* Price for CO_2 emission certificates does not rise (C) *During the process:* /	*At the start:* / *During the process:* Conduct research project: Overregulation prevents innovation (e.g., regulations) Political decisions must provide long-term security (broad acceptance)
Economic	*At the start:* Financial viability and competitiveness compared to other solutions (C) *During the process:* /	*At the start:* Pre-assessment of costs at an early stage (TRL 1–3) *During the process:* /	*At the start:* Financial viability and competitiveness compared to other solutions (C) *During the process:* /	*At the start:* / *During the process:* Linking technical assessment with costs	*At the start:* Financial viability and competitiveness compared to other solutions (biomass, cheap oil-based materials) (C) Competition with oil industry (B) *During the process:* Starting materials might not be available at the required scale (B) Too expensive? (R)	*At the start:* Cost assessment *During the process:* Forecasting not only CO_2 price but other prices too Business models (also in changing contexts) Estimations, data generation (data is existing, e.g., how much biodiesel is produced) To decrease by-product content of final product with this price of final product and limitations Alternatives for biodiesel by-product such as cheaper alcohols regarding biodiesel industry will be less

Note. C = Challenges, B = Barriers, R = Risks, Umweltbundesamt = German government environmental agency, BASt = German Federal Highway Research Institute.[1]This element is categorised in both environmental and human health considerations.

Data availability

No data was used for the research described in the article.

References

Abbate, E., Garmendia Aguirre, I., Bracalente, G., Mancini, L., Tosches, D., Rasmussen, K., Bennett, M.J., Rauscher, H., Sala, S., 2024. Safe and Sustainable by Design Chemicals and Materials: Methodological Guidance. Publications Office of the European Union. https://doi.org/10.2760/28450.

Aicardi, C., Fothergill, B.T., Rainey, S., Stahl, B.C., Harris, E., 2018. Accompanying technology development in the Human Brain Project: from foresight to ethics management. Futures 102, 114–124. https://doi.org/10.1016/j.futures.2018.01.005.

American Chemical Society, 2024a. 12 principles of green chemistry. https://www.acs.org/greenchemistry/principles/12-principles-of-green-chemistry.html.

American Chemical Society, 2024b. Green chemistry history. https://www.acs.org/greenchemistry/what-is-green-chemistry/history-of-green-chemistry.html.

Amir, O., 2013. A topology optimization procedure for reinforced concrete structures. Comput. Struct. 114–115, 46–58. https://doi.org/10.1016/j.compstruc.2012.10.011.

Anastas, P.T., Eghbali, N., 2010. Green chemistry: principles and practice. Chem. Soc. Rev. 39 (1), 301–312. https://doi.org/10.1039/B918763B.

Anastas, P.T., Williamson, T.C. (Eds.), 1996. Green Chemistry: Designing Chemistry for the Environment. ACS Symposium Series, vol. 626. American Chemical Society. https://doi.org/10.1021/bk-1996-0626.

Blum, C., Bunke, D., Hungsberg, M., Roelofs, E., Joas, A., Joas, R., Blepp, M., Stolzenberg, H.-C., 2017. The concept of sustainable chemistry: key drivers for the transition towards sustainable development. Sustainable Chemistry and Pharmacy 5, 94–104. https://doi.org/10.1016/j.scp.2017.01.001.

Caldeira, C., Farcal, L.R., Garmendia Aguirre, I., Mancini, L., Tosches, D., Amelio, A., Rasmussen, K., Rauscher, H., Riego Sintes, J., Sala, S., 2022. Safe and sustainable by design chemicals and materials. Framework for the definition of criteria and evaluation procedure for chemicals and materials. https://doi.org/10.2760/487955.

Castilla-Polo, F., Sánchez-Hernández, M.I., 2022. International orientation: an antecedent-consequence model in Spanish agri-food cooperatives which are aware of the circular economy. J. Bus. Res. 152, 231–241. https://doi.org/10.1016/j.jbusres.2022.07.038.

Chen, T.-L., Kim, H., Pan, S.-Y., Tseng, P.-C., Lin, Y.-P., Chiang, P.-C., 2020. Implementation of green chemistry principles in circular economy system towards sustainable development goals: challenges and perspectives. Sci. Total Environ. 716, 136998. https://doi.org/10.1016/j.scitotenv.2020.136998.

Cordella, M., Horn, R., Hong, S.H., Bianchi, M., Isasa, M., Harmens, R., et al., 2023. Addressing sustainable development goals in life cycle sustainable assessment: synergies, challenges and needs. J. Clean. Prod. 415, 137719. https://doi.org/10.1016/j.jclepro.2023.137719.

Eggen, R.I.L., Hollender, J., Joss, A., Schärer, M., Stamm, C., 2014. Reducing the discharge of micropollutants in the aquatic environment: the benefits of upgrading wastewater treatment plants. Environmental Science & Technology 48 (14), 7683–7689. https://doi.org/10.1021/es500907n.

European Environmental Bureau, 2017. Keeping it clean: how to protect the circular economy from hazardous substances. https://eeb.org/library/keeping-it-clean-how-to-protect-the-circular-economy-from-hazardous-substances/.

Eurostat, 2024. Waste statistics: total waste generation. https://ec.europa.eu/eurostat/statistics-explained/index.php?title=Waste_statistics#Total_waste_generation.

Falcone, P.M., Hiete, M., 2019. Exploring green and sustainable chemistry in the context of sustainability transition: the role of visions and policy. Curr. Opin. Green Sustainable Chem. 19, 66–75. https://doi.org/10.1016/j.cogsc.2019.08.002.

Flipse, S.M., van der Sanden, M.C., Osseweijer, P., 2014. Improving industrial R&D practices with social and ethical aspects: aligning key performance indicators with social and ethical aspects in food technology R&D. Technol. Forecast. Soc. Change 85, 185–197. https://doi.org/10.1016/j.techfore.2013.08.009.

Ganesh, K.N., Zhang, D., Miller, S.J., Rossen, K., Chirik, P.J., Kozlowski, M.C., Zimmerman, J.B., Brooks, B.W., Savage, P.E., Allen, D.T., Voutchkova-Kostal, A.M., 2021. Green chemistry: a framework for a sustainable future. Organometallics 40 (12), 1801–1805. https://doi.org/10.1021/acs.organomet.1c00343.

Garcia Martinez, J., 2016. Tackling the big challenges of the future. Chem. Int. 38 (3–4). https://doi.org/10.1515/ci-2016-3-405.

Gerrits, E.M., Bredenoord, A.L., van Mil, M.H., 2022. Educating for responsible research practice in biomedical sciences: towards learning Goals. Sci. Educ. 31 (4), 977–996. https://doi.org/10.1007/s11191-021-00295-y.

Hearn, J.D., Weber, R., Nichols, R., Henley, M.V., Fox, S., 2013. Deposition of Cl2 on soils during outdoor releases. J. Hazard Mater. 252–253, 107–114. https://doi.org/10.1016/j.jhazmat.2013.02.038.

Horváth, I.T., Anastas, P.T., 2007a. Innovations and green chemistry. Chem. Rev. 107 (6), 2169–2173. https://doi.org/10.1021/cr078380v.

Horváth, I.T., Anastas, P.T., 2007b. Introduction: green chemistry. Chem. Rev. 107 (6), 2167–2168. https://doi.org/10.1021/cr0783784.

Leso, V., Rydberg, T., Halling, M., Karakitsios, S., Nikiforou, F., Karakoltzidis, A., et al., 2024. Safety and sustainability by design: an explorative survey on concepts' knowledge and application. Environ. Sci. Pol. 162, 103909. https://doi.org/10.1016/j.envsci.2024.103909.

Li, M., Kühlen, A., Yang, J., Schultmann, F., 2013. Improvement of the statutory framework for construction and demolition waste management exemplified in Germany and Australia. In: Rauch, S., Morrison, G., Norra, S., Schleicher, N. (Eds.), Urban Environment: Proceedings Of the 11th Urban Environment Symposium (UES), Held in Karlsruhe, Germany, 16-19 September 2012. Springer, Springer Netherlands; Imprint, pp. 15–25. https://doi.org/10.1007/978-94-007-7756-9_2.

Lin, R., Amrute, A.P., Pérez-Ramírez, J., 2017. Halogen-mediated conversion of hydrocarbons to commodities. Chem. Rev. 117 (5), 4182–4247. https://doi.org/10.1021/acs.chemrev.6b00551.

Linder, M., 2017. Ripe for disruption: reimagining the role of green chemistry in a circular economy. Green Chem. Lett. Rev. 10 (4), 428–435. https://doi.org/10.1080/17518253.2017.1392618.

Loste, N., Roldán, E., Giner, B., 2020. Is Green Chemistry a feasible tool for the implementation of a circular economy? Environ. Sci. Pollut. Control Ser. 27 (6), 6215–6227. https://doi.org/10.1007/s11356-019-07177-5.

Luo, Y., Guo, W., Ngo, H.H., Nghiem, L.D., Hai, F.I., Zhang, J., Liang, S., Wang, X.C., 2014. A review on the occurrence of micropollutants in the aquatic environment and their fate and removal during wastewater treatment. Sci. Total Environ. 473–474, 619–641. https://doi.org/10.1016/j.scitotenv.2013.12.065.

Manley, J.B., Anastas, P.T., Cue, B.W., 2008. Frontiers in green chemistry: meeting the grand challenges for sustainability in R&D and manufacturing. J. Clean. Prod. 16 (6), 743–750. https://doi.org/10.1016/j.jclepro.2007.02.025.

Martin, M.T., Judson, R.S., Reif, D.M., Kavlock, R.J., Dix, D.J., 2009. Profiling chemicals based on chronic toxicity results from the U.S. Epa ToxRef Database. Environmental Health Perspectives 117 (3), 392–399. https://doi.org/10.1289/ehp.0800074.

Mehlich, J., 2018. Chemistry and dual use: from scientific integrity to social responsibility. Helv. Chim. Acta 101 (9), e1800098. https://doi.org/10.1002/hlca.201800098.

Mehlich, J., 2023. Responsible chemistry. Chem. Int. 45 (3), 12–15. https://doi.org/10.1515/ci-2023-0303.

Murray, A., Skene, K., Haynes, K., 2017. The circular economy: an interdisciplinary exploration of the concept and application in a global context. J. Bus. Ethics 140, 369–380. https://doi.org/10.1007/s10551-015-2693-2.

Neuberger, S., Paier, M., Hörlesberger, M., 2024. The effects of RRI-oriented roadmapping on the digital transformation of regions. Journal of Responsible Innovation 11 (1), 2414519. https://doi.org/10.1080/23299460.2024.2414519.

Owen, R., Goldberg, N., 2010. Responsible innovation: a pilot study with the U.K. Engineering and physical sciences research council. Risk Anal. 30 (11), 1699–1707. https://doi.org/10.1111/j.1539-6924.2010.01517.x.

Owen, R., Stilgoe, J., Macnaghten, P., Gorman, M., Fisher, E., Guston, D., 2013. A framework for responsible innovation. In: Responsible Innovation. John Wiley & Sons, Ltd, pp. 27–50. https://doi.org/10.1002/9781118551424.ch2.

Park, H., Phaal, R., Ho, J.-Y., O'Sullivan, E., 2020. Twenty years of technology and strategic roadmapping research: a school of thought perspective. Technol. Forecast. Soc. Change 154, 119965. https://doi.org/10.1016/j.techfore.2020.119965.

Porcari, A., Pimponi, D., Borsella, E., Mantovani, E., 2019. PRISMA RRI-CSR roadmap: deliverable 5.2 - Part A. https://www.rri-prisma.eu/wp-content/uploads/2019/06/PRISMA_RRI_Exemplar_Roadmap_June-_2019.pdf.

Roh, K., Brée, L.C., Perrey, K., Bulan, A., Mitsos, A., 2019. Flexible operation of switchable chlor-alkali electrolysis for demand side management. Appl. Energy 255, 113880. https://doi.org/10.1016/j.apenergy.2019.113880.

Schneider, C., Roßmann, M., Lösch, A., Grunwald, A., 2021. Transformative vision assessment and 3-D printing futures: a new approach of technology assessment to address grand societal challenges. IEEE Trans. Eng. Manag. 70 (3), 1089–1098. https://doi.org/10.1109/TEM.2021.3129834.

Schwarzenbach, R.P., Escher, B.I., Fenner, K., Hofstetter, T.B., Johnson, C.A., Gunten, U. von, Wehrli, B., 2006. The challenge of micropollutants in aquatic systems. Science (New York, N.Y.) 313 (5790), 1072–1077. https://doi.org/10.1126/science.1127291.

Shelley-Egan, C., Bowman, D.M., Robinson, D.K.R., 2018. Devices of responsibility: over a decade of responsible research and innovation initiatives for nanotechnologies. Sci. Eng. Ethics 24 (6), 1719–1746. https://doi.org/10.1007/s11948-017-9978-z.

Silvestri, C., Silvestri, L., Forcina, A., Di Bona, G., Falcone, D., 2021. Green chemistry contribution towards more equitable global sustainability and greater circular economy: a systematic literature review. J. Clean. Prod. 294, 126137. https://doi.org/10.1016/j.jclepro.2021.126137.

Stahl, B.C., Chatfield, K., Ten Holter, C., Brem, A., 2019. Ethics in corporate research and development: can responsible research and innovation approaches aid sustainability? J. Clean. Prod. 239, 118044. https://doi.org/10.1016/j.jclepro.2019.118044.

Stahl, B.C., Eden, G., Jirotka, M., Coeckelbergh, M., 2014. From computer ethics to responsible research and innovation in ICT: the transition of reference discourses informing ethics-related research in information systems. Inf. Manag. 51 (6), 810–818. https://doi.org/10.1016/j.im.2014.01.001.

Stilgoe, J., Owen, R., Macnaghten, P., 2013. Developing a framework for responsible innovation. Res. Pol. 42 (9), 1568–1580. https://doi.org/10.1016/j.respol.2013.05.008.

European Commission, Directorate-General for Research and Innovation, Strazza, C., Olivieri, N., De Rose, A., et al., European Commission, Directorate-General for Research and Innovation, 2017. Technology readiness level - Guidance principles for renewable energy technologies - Final report. Publications Office. https://data.europa.eu/doi/10.2777/577767.

Tassone, V.C., O'Mahony, C., McKenna, E., Eppink, H.J., Wals, A.E., 2018. (Re-)designing higher education curricula in times of systemic dysfunction: a responsible research and innovation perspective. High Educ. 76, 337–352. https://doi.org/10.1007/s10734-017-0211-4.

Thapa, R.K., Iakovleva, T., Foss, L., 2019. Responsible research and innovation: a systematic review of the literature and its applications to regional studies. Eur. Plann. Stud. 27 (12), 2470–2490. https://doi.org/10.1080/09654313.2019.1625871.

Timmermans, J., 2017. Mapping the RRI landscape: an overview of organisations, projects, persons, areas and topics. In: Asveld, L., van Dam-Mieras, R., Swierstra, T., Lavrijssen, S., Linse, K., van den Hoven, J. (Eds.), Responsible Innovation 3. A European Agenda? Springer International Publishing, pp. 21–47. https://link.springer.com/chapter/10.1007/978-3-319-64834-7_3.

United Nations Environment Programme, 2019. Global Chemicals Outlook II: from legacies to innovative solutions. UN Environment Programme. https://www.unep.org/resources/report/global-chemicals-outlook-ii-legacies-innovative-solutions.

von Schomberg, R., 2012. Prospects for technology assessment in a framework of responsible research and innovation. In: Dusseldorp, M., Beecroft, R. (Eds.), Technikfolgen Abschätzen Lehren: Bildungspotenziale Transdisziplinärer Methoden. VS Verlag für Sozialwissenschaften. https://doi.org/10.1007/978-3-531-93468-6_2.

Winder, C., 2001. The toxicology of chlorine. Environ. Res. 85 (2), 105–114. https://doi.org/10.1006/enrs.2000.4110.

References for Appendix A

Anastas, P.T., Williamson, T.C. (Eds.), 1996. *Green chemistry: Designing chemistry for the environment*. American chemical society. ACS symposium series 626. https://doi.org/10.1021/bk-1996-0626.

Castilla-Polo, F., Sánchez-Hernández, M.I., 2022. International orientation: anantecedent-consequence model in Spanish agri-food cooperatives which are aware ofthe circular economy. J. Bus. Res. 152, 231–241. https://doi.org/10.1016/j.jbusres.2022.07.038.

Clarivate, 2023. Citing Journal Citation Reports. Journal Citation Reports. https://jcr.help.clarivate.com/Content/citing-jcr.html.

Inigo, E.A., Blok, V., 2019. Strengthening the socio-ethical foundations of the circular economy: lessons from responsible research and innovation. J. Clean. Prod. 233, 280–291. https://doi.org/10.1016/j.jclepro.2019.06.053.

MacArthur, E., 2013. Towards the circular economy. J. Ind. Ecol. 2 (1), 23–44. https://www.ellenmacarthurfoundation.org/towards-the-circular-economy-vol-1-an-economic-and-business-rationale-for-an.

Owen, R., Stilgoe, J., Macnaghten, P., Gorman, M., Fisher, E., Guston, D., 2013. A framework for responsible innovation. In: Responsible Innovation. John Wiley & Sons, Ltd, pp. 27–50. https://doi.org/10.1002/9781118551424.ch2.

Page, M.J., McKenzie, J.E., Bossuyt, P.M., Boutron, I., Hoffmann, T.C., Mulrow, C.D., Shamseer, L., Tetzlaff, J.M., Akl, E.A., Brennan, S.E., Chou, R., Glanville, J., Grimshaw, J.M., Hróbjartsson, A., Lalu, M.M., Li, T., Loder, E.W., Mayo-Wilson, E., McDonald, S., Moher, D., 2021. The PRISMA 2020 statement: an updated guideline for reporting systematic reviews. BMJ 372, n71. https://doi.org/10.1136/bmj.n71.

Parada, M.P., Kehrein, P., Xevgenos, D., Asveld, L., Osseweijer, P., 2022. Societal values, tensions and uncertainties in resource recovery from wastewaters. J. Environ. Manag. 319, 115759. https://doi.org/10.1016/j.jenvman.2022.115759.

Rethlefsen, M.L., Kirtley, S., Waffenschmidt, S., Ayala, A.P., Moher, D., Page, M.J., Koffel, J.B., 2021. Prisma-S: an extension to the PRISMA statement for reporting literature searches in systematic reviews. Syst. Rev. 10 (1), 39. https://doi.org/10.1186/s13643-020-01542-z.

Purvis, B., Celebi, D., Pansera, M., 2023. A framework for a responsible circular economy. J. Clean. Prod. 400, 136679. https://doi.org/10.1016/j.jclepro.2023.136679.

Stilgoe, J., Owen, R., Macnaghten, P., 2013. Developing a framework for responsible innovation. Res. Pol. 42 (9), 1568–1580. https://doi.org/10.1016/j.respol.2013.05.008.