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ANÁLISE DA SUSTENTABILIDADE DO CICLO DE VIDA DO NANOFERRO NA REMEDIAÇÃO DE ÁREAS CONTAMINADAS

Caroline Visentin

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ANÁLISE DA SUSTENTABILIDADE DO CICLO DE VIDA DO NANOFERRO NA REMEDIAÇÃO DE ÁREAS CONTAMINADAS

Caroline Visentin

Tese de Doutorado apresentada ao Programa de Pós-Graduação em Engenharia Civil e Ambiental da Faculdade de Engenharia e Arquitetura da Universidade de Passo Fundo, como requisito para obtenção do título de Doutora, sob a orientação do Prof. Dr. Antônio Thomé.

Comissão Examinadora:

Prof. Dr. Antônio Thomé

Universidade de Passo Fundo – UPF

Orientador

Prof. Dr. Pedro Domingos Marques Prietto

Universidade de Passo Fundo – UPF

Prof. Dra. Luciana Londero Brandli

Universidade de Passo Fundo – UPF

Prof. Dra. Cassia Maria Lie Ugaya

Universidade Tecnológica Federal do Paraná - UTFPR

Prof. Dra. Ana Carolina Badalotti Passuello

Universidade Federal do Rio Grande do Sul - UFRGS

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RESUMO

A sustentabilidade tornou-se um fator chave nas últimas décadas. Inúmeros métodos foram desenvolvidos para avaliar a sustentabilidade, como o caso da Avaliação da Sustentabilidade do Ciclo de Vida (ASCV). Enquanto que, o uso de nanomateriais na remediação vem crescendo ao longo dos anos, e o nanoferro (nFeZ) é o mais utilizado. Deste modo, o objetivo deste trabalho é avaliar a sustentabilidade do ciclo de vida do nanoferro na remediação de áreas contaminadas. Para alcançar o objetivo dividiu-se o escopo da pesquisa em quatro etapas principais: (1) avaliação da sustentabilidade do ciclo de vida da produção do nFeZ, sendo avaliado nove métodos de produção do nFeZ; (2) a avaliação da sustentabilidade do ciclo de vida da aplicação do nFeZ na remediação de áreas contaminadas, através da análise de cinco estudos de caso de abrangência mundial em diferentes configurações; (3) análise de viabilidade do uso do nFeZ na remediação de áreas contaminadas no Brasil, comparando com as técnicas tradicionais de remediação mais usadas no país; estas três etapas envolvem a aplicação da Avaliação do Ciclo de Vida (ACV), Custo do Ciclo de Vida (CCV), Avaliação do Ciclo de Vida Social (ACV-Social) e Avaliação da Sustentabilidade do Ciclo de Vida (ASCV; (4) e por fim, foi elaborado um método de agregação dos resultados das análises do ciclo de vida da ASCV, através de um índice composto de sustentabilidade. O método final foi definido com base em uma análise de diferentes métodos utilizados na agregação dos resultados das análises do ciclo de vida e também considerando a participação de pesquisadores na área para determinar a importância de diferentes critérios de seleção destes métodos de agregação. Assim, o método proposto consiste na otimização de métodos de agregação, considerando uma pontuação e escala de classificação da sustentabilidade. De forma geral, é possível destacar que os resultados obtidos dão consistência ao estudo e indicam a sua relevância. Este estudo preenche em todas suas etapas importantes lacunas científicas, contribuindo com o estado da arte para a área da remediação sustentável, do nFeZ e da ASCV. Conclui-se que o uso do nFeZ na remediação pode não ser sustentável, e considerando a perspectiva do Brasil, importantes configurações são necessárias. Além disso, o método de ASCV proposto proporciona uma análise consistente, suprindo as limitações dos métodos de agregação existentes e facilitando e contribuindo com o processo de análise da sustentabilidade.

Palavras-chaves: Nanoremediação; Remediação sustentável; Avaliação do Ciclo de Vida (ACV); Avaliação do Ciclo de Vida Social (ACV-S); Avaliação do Custo do Ciclo de Vida (CCV); Avaliação da Sustentabilidade do Ciclo de Vida (ASCV).

ABSTRACT

Sustainability has become a key factor in recent decades. Numerous methods have been developed to assess sustainability, such as the Life Cycle Sustainability Assessment (LCSA). While, the use of nanomaterials in remediation has been growing over the years, and nano scale zero valent iron (nZVI) is the most widely used. Thus, the aim of this work is to evaluate the sustainability of the life cycle of nZVI in the remediation of contaminated sites. To achieve the objective, the scope of the research was divided into four main stages: (1) evaluation of the sustainability of the life cycle of nZVI production, being evaluated nine methods of nZVI production; (2) the evaluation of the sustainability of the life cycle of the application of nZVI in the remediation of contaminated areas, through the analysis of five case studies of worldwide coverage in different configurations; (3) feasibility analysis of the use of nZVI in the remediation of contaminated areas in Brazil, comparing with the most used traditional remediation techniques in the country; these three steps involve the application of life cycle assessment (LCA), Life Cycle Cost (LCC), Social Life Cycle Assessment (S-LCA) and Life Cycle Sustainability Assessment (LCSA); (4) and finally, a method of aggregation of the results of the life cycle analyses of the LCSA was elaborated, through a composite index of sustainability. The final method was defined based on an analysis of different methods used in the aggregation of the results of life cycle analyses and also considering the participation of researchers in the area to determine the importance of different selection criteria of these aggregation methods. Thus, the proposed method consists in the optimization of aggregation methods, considering a score and scale of sustainability classification. In general, it is possible to highlight that the results obtained give consistency to the study and indicate its relevance. This study fills in all its stages important scientific gaps, contributing to the state of the art for the area of sustainable remediation, nZVI and LCSA. It is concluded that the use of nZVI in remediation may not be sustainable, and considering the perspective of Brazil, important configurations are necessary. In addition, the proposed LCSA method provides a consistent analysis, meeting the limitations of existing aggregation methods and facilitating and contributing to the sustainability analysis process.

Keywords: Nanoremediation; Sustainable remediation; Life cycle assessment (LCA); Social life cycle assessment (S-LCA); Life cycle cost assessment (LCC); Life cycle sustainability assessment (LCSA).

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1 INTRODUÇÃO GERAL

O desenvolvimento sustentável está se tornando cada vez mais importante para apoiar a tomada de decisões de políticas empresariais e governamentais (RODRIGUES et al. 2020). Em 2015, as Nações Unidas desenvolveram os Objetivos de Desenvolvimento Sustentável (ODS), compreendendo 17 objetivos e 169 metas de integração de questões relacionadas ao desenvolvimento sustentável nas estruturas econômicas, ambientais e sociais gerais dos países (CAIADO et al. 2018; SALVIA et al., 2019a). Os ODS são um objetivo global com prioridades e aspirações para alcançar o desenvolvimento sustentável para 2030. Os 17 objetivos desenvolvidos compreendem diversas áreas como saúde, educação, segurança, meio ambiente, igualdade de gênero, cidades e infraestrutura (MCARTHUR; RASMUSSEN, 2018, LEAL FILHO et al., 2018).

Para que o desenvolvimento sustentável seja implementado de forma eficaz, são necessárias medidas de avaliação da sustentabilidade. A estrutura da avaliação de sustentabilidade é baseada em: (i) dados de inventário, ou seja, indicadores e índices; (ii) ferramentas de avaliação relacionadas ao produto com foco nos fluxos de material e/ou energia de um produto ou serviço, como, por exemplo, avaliação do ciclo de vida; e (iii) avaliação integrada, que é um conjunto de ferramentas geralmente focadas na mudança de políticas ou na implementação de projetos (por exemplo: ferramentas de análise multicritérios, análise de riscos, análise de custo benefício) (SINGH et al. 2012; SALA et al., 2015).

Neste contexto tem-se a Análise da Sustentabilidade do Ciclo de Vida (ASCV) como uma forma de avaliação da sustentabilidade de produtos, serviços e organizações em um contexto de ciclo de vida através de uma abordagem mais holística da sustentabilidade (EKENER et al., 2018; WAFA et al. 2022). A ASCV originalmente foi estruturada de acordo com os três pilares da sustentabilidade e respectivas análises do ciclo de vida, ou seja, Avaliação do ciclo de Vida (ACV) (ISO, 2006), Custo do Ciclo de vida (CCV) (SETAC, 2011) e Avaliação do ciclo de Vida Social (ACV-Social) (KLOEPFFER, 2008; UNEP 2009, 2020). A inclusão dos conceitos do desenvolvimento sustentável em uma abordagem de ciclo de vida garante que os aspectos de sustentabilidade sejam levados em consideração ao longo de todo o ciclo de vida do sistema que está sendo considerado (KLOEPFFER, 2008).

Como uma ferramenta de avaliação da sustentabilidade, a ASCV ajuda organizações, indústrias e países a atingir seus objetivos com vistas ao desenvolvimento sustentável e ao serviço dos ODS. A análise mais ampla da ASCV abrange os ODS em sua avaliação e, portanto, é uma ferramenta importante para ajudar as organizações, setores econômicos, e indústrias a identificar os impactos ambientais, sociais e econômicos de suas atividades a partir de uma perspectiva de ciclo de vida (REN et al., 2015; VAN KEMPEN et al., 2017).

A inclusão da sustentabilidade em inúmeras áreas de estudo faz com que ocorra o surgimento de novas áreas de pesquisas e o desenvolvimento de métodos e ferramentas para auxiliar os tomadores de decisão considerando os aspectos da sustentabilidade nesse processo. Neste sentido, ao longo das últimas décadas, houve um acréscimo gradual na preocupação com a sustentabilidade dos processos de remediação, devido à preocupação com os impactos e benefícios que a remediação pode causar. A disseminação da remediação sustentável fez com que a preocupação não seja apenas a descontaminação, esta abordagem é mais ampla e considera os impactos ambientais, econômicos e sociais do ciclo de vida dos processos de remediação (EIZENBERG et al. 2017; BRAUN et al. 2019b).

Entretanto, o crescimento da demanda por processos de remediação, a fim de suprir a necessidade de descontaminação de áreas contaminadas, ocasionou o aumento do número de estudos e discussões sobre novas técnicas e materiais de remediação, como, por exemplo, o uso de nanomateriais, como o caso do nanoferro. Muitas das técnicas tradicionais de remediação acabam resultando em elevados consumos de recursos, além de demandarem maiores tempos para a remediação. Deste modo, existem fortes incentivos para considerar processos alternativos e inovadores de remediação (PHENRAT; LOWRY; BABAKHANI, 2019).

O uso de nanomateriais na remediação ambiental vem com a finalidade de fornecer uma técnica com alta eficiência, menor tempo de tratamento, melhores custos e benefícios, além de poder ser empregada em locais contaminados com vários tipos de substâncias (THOMÉ et al. 2015). Dentre os nanomateriais empregados na remediação, destaca-se o ferro nano escala zero valente (nFeZ) (CECCHIN et al. 2016). O nFeZ é um dos nanomateriais mais estudados para uso na remediação ambiental ao longo dos últimos 20 anos (ZHAO et al. 2016), e também é o mais empregado em processos de nanoremediação de solos nos Estados Unidos, correspondendo a 47% das aplicações (EPA 2010). Seu uso extensivo é atribuído à sua eficiência de remoção, sua praticidade na injeção nos ambientes subsuperficiais devido a sua baixa toxicidade e custo de produção (THOMÉ et al. 2015; GIL-DÍAZ et al. 2017).

Entretanto, a sustentabilidade destes novos processos deve ser avaliada de forma a verificar se a tecnologia a ser utilizada supre também com as melhorias dos aspectos ambientais, econômicos e sociais. Assegurar o desenvolvimento sustentável e a utilização de nFeZ para remediação requer a incorporação de múltiplos fatores e critérios, incluindo os relacionados com o desempenho tecnológico; custos; potenciais impactos para o ambiente e a saúde humana, considerando todo o seu ciclo de vida (GRIEGER et al., 2019). Portanto, diversos grupos de *stakeholders*, incluindo agências governamentais, universidades, institutos de pesquisa e indústria, estão interessados em maneiras pelas quais o nFeZ pode ser desenvolvido e utilizado de forma sustentável. Para que o nFeZ seja uma tecnologia competitiva as considerações ambientais, econômicas e sociais devem ser incluídas no desenvolvimento e implantação do nFeZ, juntamente com os aspectos de tomada de decisão em todo o ciclo de vida deste nanomaterial, desde a sua produção até a utilização na remediação (PHENRAT; LOWRY; BABAKHANI, 2019).

O uso do nFeZ na remediação ainda é pouco explorado em relação à análise de impacto. Até o momento, apenas um estudo avaliou a sustentabilidade do uso do nFeZ na remediação, usando dados do projeto NanoRem realizado pelo Quadro da Comissão Europeia (de 2013 ao início de 2017) (BONE et al. 2020). Os autores utilizaram uma pasta de trabalho NanoRem para avaliação de sustentabilidade, um processo que avalia a sustentabilidade por meio de três etapas: preparação, definição e execução. A avaliação é feita qualitativamente, definindo pontuações para cada aspecto de sustentabilidade avaliado. Em comparação com as demais técnicas avaliadas (oxidação química in situ, nanorremediação integrada in situ com corrente contínua e escavação e eliminação), a nanorremediação foi favorável. No entanto, ainda há lacunas a serem preenchidas e, até o momento, não há nenhum estudo que avalie a sustentabilidade do ciclo de vida do uso do nFeZ na remediação de locais contaminados.

Além disso, em relação a ASCV até o momento não há um método universal aceito pela comunidade científica. Esta lacuna vem sendo destacada em inúmeros estudos. Valdívia et al. (2020) destaca que a estrutura ASCV é globalmente aceita e a necessidade de uma abordagem aplicável está aumentando constantemente. Gubert (2017) argumenta que a ASCV precisa de uma maneira explícita e padronizada de integrar as preferências nas categorias de impacto ambiental, social e econômico. Alejandrino et al. (2021) destacam a necessidade de fortalecer os *trade-offs* metodológicos e obter uma base consistente para futuros estudos de caso de ASCV. Portanto, são necessários métodos que promovam a agregação dos resultados da avaliação do ciclo de vida na

ASCV de forma simples e orientativas, a fim de melhorar a tomada de decisão na sustentabilidade de produtos, serviços e processos (Visentin et al. 2020).

A partir destas realidades, o principal problema que direciona a temática investigada está ancorado nas seguintes questões: Qual a sustentabilidade dos diferentes métodos de produção do nFeZ? O uso do nanoferro em processos de remediação em um cenário mundial é sustentável? E considerando a realidade brasileira, o uso do nanoferro é sustentável? E ainda, como criar um método de ASCV que integre os elementos essenciais que ajudam o tomador de decisão a maximizar o tempo na avaliação da sustentabilidade do ciclo de vida?

Esta pesquisa justifica-se pelo fato de que nos últimos anos mais atenção tem se dado à questão da sustentabilidade, seja ela na remediação de áreas contaminadas como também na avaliação do ciclo de vida. E juntamente com esta preocupação, tem crescido no cenário mundial o reconhecimento da importância da incorporação dos elementos de sustentabilidade na tomada de decisão (BRAUN, 2021). A sustentabilidade tornou-se um fator-chave no desenvolvimento de grandes corporações e cidades, devido ao desenvolvimento sustentável gerar benefícios para a sociedade no todo.

Com o crescente interesse em alcançar a sustentabilidade global, mais estudos estão introduzindo o conceito de sustentabilidade e as ferramentas de avaliação da sustentabilidade para sistemas estratégicos de tomada de decisão, a fim de melhorar o desempenho da sustentabilidade dos produtos (HANNOUF e ASSEFA, 2018). Para avançar em direção ao desenvolvimento sustentável, é necessária uma abordagem mais holística da sustentabilidade (EKENER et al., 2018). Neste contexto, percebe-se que a aplicação da ASCV tem vindo a aumentar nos últimos anos (VISENTIN et al. 2020).

De forma complementar, outro aspecto que justifica esta pesquisa está relacionado com a necessidade, elencada na literatura, de conhecer os impactos ambientais, econômicos e sociais associados ao ciclo de vida do nFeZ. Assim, esta pesquisa busca preencher esta lacuna científica, avaliando de forma conjunta, os impactos ambientais, sociais e econômicos do ciclo de vida resultantes dos métodos de produção do nFeZ e da sua aplicação na remediação.

Como ferramenta de suporte à decisão, a avaliação da sustentabilidade do ciclo de vida fornece uma visão geral do desempenho de sustentabilidade dos sistemas de produção, destacando áreas de impacto negativo significativo, onde melhorias podem ser feitas, e as oportunidades que podem ser exploradas (GBEDEDO; LIYANAGE; GARZA-REYES, 2018; KABAYO et al., 2019). Além disso, a ASCV pode ser usada na melhoria da sustentabilidade de um determinado sistema, como o nFeZ, por exemplo, e também como fonte de vantagem competitiva para empresas e organizações (ROINIOTI; KORONEOS, 2019; SETTEMBRE BLUNDO et al., 2019). A busca da empresa, indústria e organizações para uma ampla avaliação de sustentabilidade como a ASCV também beneficia em seu compromisso com os ODSs (WANG et al., 2018).

Portanto, o conhecimento da sustentabilidade das técnicas de remediação e dos materiais empregados na remediação torna-se um importante aliado dos tomadores de decisão na escolha das melhores alternativas de remediação para determinado local, considerando os aspectos ambientais, sociais e econômicos. Com o crescente avanço do conceito de remediação sustentável, e do uso da nanotecnologia e do nFeZ na remediação de solos, torna-se necessário empregar mecanismos de avaliação da sustentabilidade desta tecnologia, para assim, orientar os tomadores de decisão, as empresas fabricantes, a sociedade e os trabalhadores sobre o ciclo de vida do nFeZ.

Além disso, a elaboração de um método de ASCV torna-se um importante aliado dos tomadores de decisão na avaliação da sustentabilidade em um contexto de ciclo de vida. O método da ASCV facilita o processo de análise, além de ser uma forma de proporcionar uma comparação adequada entre diferentes estudos, considerando a classificação de sustentabilidade proposta.

O Programa de Pós-graduação em Engenharia Civil e Ambiental, em sua linha de pesquisa Infraestrutura Sustentável através do grupo de Pesquisa em Geotecnia Ambiental, no qual este estudo está inserido, tem desenvolvido diversos trabalhos voltados para a remediação de áreas contaminadas com o uso do nFeZ e também na área da remediação sustentável.

As pesquisas relacionando os aspectos da sustentabilidade do nFeZ vem crescendo devido principalmente às publicações do grupo de pesquisa de Geotecnia Ambiental da Universidade de Passo Fundo na linha de pesquisa da Remediação Sustentável. Até o momento seis estudos que avaliaram os impactos ambientais e custos de métodos de síntese do nFeZ (MARTINS et al. 2017; JOSHI et al., 2018; VISENTIN et al., 2019), os impactos sociais (VISENTIN et al. 2022a) e a sustentabilidade (VISENTIN et al. 2021a; 2022b). As publicações do grupo de pesquisa compreendem aos resultados do mestrado da aluna Caroline Visentin e também resultados desta tese de doutorado (Capítulo III). As lacunas referentes à sustentabilidade dos métodos de produção do nFeZ foram preenchidas em Visentin et al. (2022b). Neste trabalho os autores avaliaram a sustentabilidade do ciclo de vida de nove métodos de produção do nFeZ identificados em Visentin et al. (2021b). Assim, esta tese dá sequência a trabalhos já realizados na linha e no grupo de pesquisa, o que contribuirá para expandir e incluir o tema e as questões da sustentabilidade do nFeZ na remediação de áreas contaminadas e também em relação a ASCV.

Portanto, as principais contribuições desta tese e o preenchimento das principais lacunas ainda existentes ancoraram-se sob quatro aspectos: (1) análise da sustentabilidade dos métodos de produção do nFeZ - até então apenas poucos estudos avaliaram aspectos da sustentabilidade dos métodos, ou apenas alguns métodos; (2) avaliação da sustentabilidade do uso do nFeZ na remediação de áreas contaminadas, demonstrando qual forma de utilização é mais sustentável; (3) análise da viabilidade do uso no nFeZ na remedição de áreas contaminadas no Brasil, uma vez que, por mais que o nFeZ seja muito pesquisado no país, ainda não se conhecia a sua sustentabilidade; (4) o desenvolvimento de um método de agregação da ASCV - até o momento não há um método de ASCV, e as tentativas para determinar este método são fundamentais.

1.1 Objetivos

Geral: avaliar a sustentabilidade do ciclo de vida do nanoferro na remediação de áreas contaminadas.

Específicos:

a) Analisar a sustentabilidade dos métodos de produção do nanoferro.
b) Avaliar a sustentabilidade da aplicação do nanoferro na remediação de áreas contaminadas.
c) Verificar a viabilidade do uso do nanoferro na remediação de solos contaminados, na perspectiva do Brasil.
d) Aplicar, avaliar e validar os métodos de agregação da ASCV de forma a propor e validar um método otimizado de agregação da ASCV.

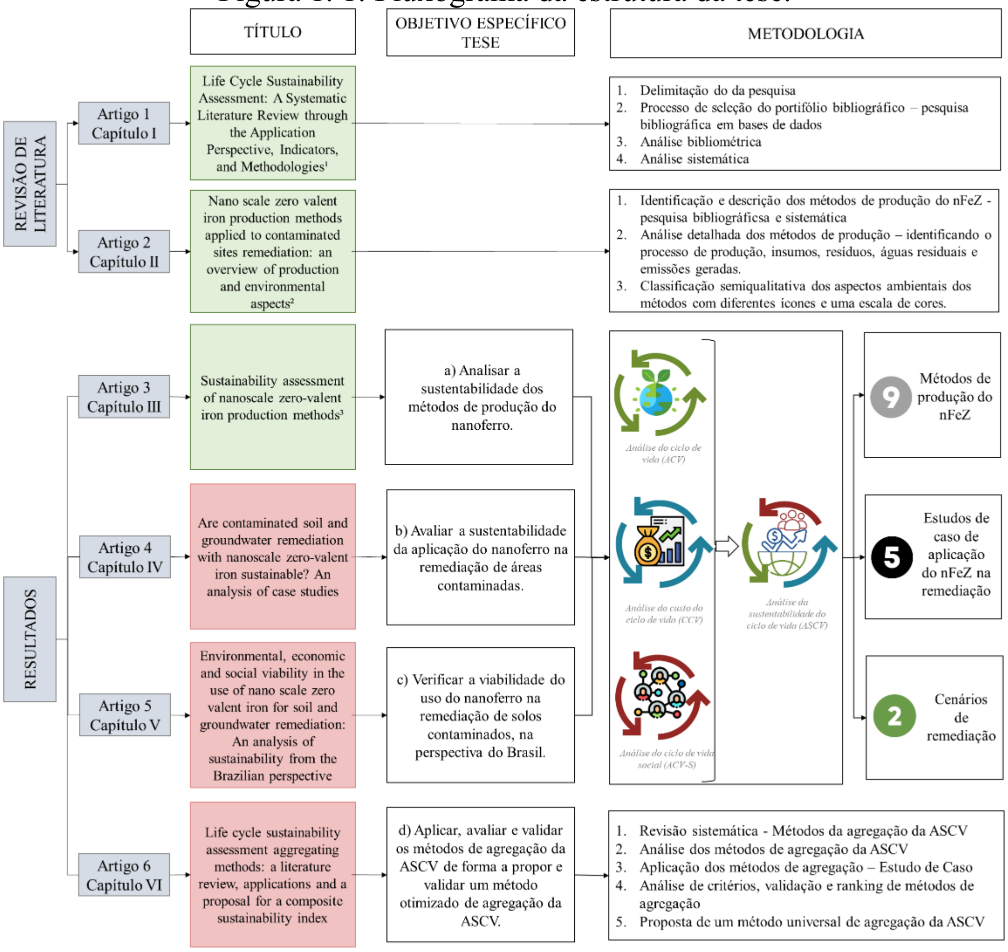
1.2 Estrutura da Tese

Este trabalho está organizado de modo que nesta introdução geral apresentou-se a contextualização do tema, a problemática, a justificativa e os objetivos da pesquisa. As seções seguintes foram organizadas em capítulos. Cada capítulo foi organizado em formato de artigo completo, com início, meio e fim, contendo as subdivisões típicas (introdução, metodologia, resultados e discussões, conclusões e referências bibliográficas). Por fim, são apresentadas as considerações e conclusões gerais e finais do trabalho, além das referências bibliográficas utilizadas na introdução geral.

A partir de todo o trabalho realizado durante o doutorado foram gerados seis artigos, dos quais três já foram publicados em renomados periódicos científicos de alto fator de impacto. Desta forma, esta tese foi dividida em seis capítulos. O primeiro capítulo corresponde ao artigo publicado de revisão bibliométrica e sistemática e está relacionado com a temática da ASCV, com enfoque na identificação dos métodos de agregação utilizados pelos estudos, indicadores de sustentabilidade e aplicação (Visentin et al. 2020).

O segundo capítulo é um artigo de revisão referente aos métodos de produção do nanoferro e dos aspectos ambientais destes métodos (Visentin et al. 2021b). Os outros quatro capítulos corresponderam aos resultados da pesquisa, os quais relacionam-se diretamente com os objetivos específicos estabelecidos e direcionados para o alcance do objetivo geral. Até o momento, houve a publicação de um dos artigos de resultados (Visentin et al. 2022), sendo que dos outros três, um foi submetido e está em revisão e os outros dois ainda não foram submetidos.

Figura 1. 1: Fluxograma da estrutura da tese.



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[3] *VISENTIN, C.; BRAUN, A. B.; TRENTIN, A. da S., THOMÉ, A. Sustainability Assessment of Nanoscale Zerovalent Iron Production Methods.* ***Environmental Engineering Science****, v. 39, n. 10, p. 847-860, 2022. https://doi.org/10.1089/ees.2021.0341*

2 CAPÍTULO I (artigo de revisão da literatura - publicado): Life Cycle Sustainability Assessment: A Systematic Literature Review through the Application Perspective, Indicators, and Methodologies[1]

Abstract

Sustainability has become a key factor in recent years. Countless methods have been developed to assess sustainability, such as the case of the Life Cycle Sustainability Analysis (LCSA). Thus, this article aims to identify and map the application of LCSA in the main scientific databases, through a process of bibliometric and systematic literature review. Therefore, a bibliographic portfolio that represents the publications of the LCSA was selected based on selection criteria, after which the bibliometric and systematic analyses were performed. The bibliometric analysis identified the temporal distribution of publications, journals, authors, and countries that contribute to the context, as well as a studies' keyword analysis. The systematic analysis was carried out by verifying the types of studies present in the bibliographic portfolio, the economic sectors and countries of applied studies localization, the indicators and methodologies used to evaluate each sustainability dimension, and the main methodologies for results final analyses were also verified. The selected bibliographic portfolio consisted of 105 publications, corresponding to the period 2008–2019. The results show that developed countries have a greater number of publications. However, China stands out with the highest number of publications. Most of the studies in the portfolio are developments of methodologies and applications in case studies. The applied studies covered several economic and global localization sectors. Moreover, it was found that there is a great variability of environmental, economic, and social indicators employed, as well as methodologies for analyzing the final results. For example, the main indicators were: eutrophication and acidification; electricity and operating and maintenance costs, and employment; and multi-criteria decision analysis (MDCA) was the most widely used methodology. This research makes several new contributions, providing academics and professionals with an overview of the application of LCSA, through scientific indexes and the main approaches of publications, as well as the perspectives of new research.

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[1] *[1] VISENTIN, C., da SILVA TRENTIN, A. W., BRAUN, A. B., THOMÉ, A. Life cycle sustainability assessment: A systematic literature review through the application perspective, indicators, and methodologies.* ***Journal of Cleaner Production****, v. 270, p. 122509, 2020. https://doi.org/10.1016/j.jclepro.2020.122509*

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1. Introduction

Sustainable development, according to the concept presented by the Brundtland Report (1987), is one that aims to meet the needs of current generations without compromising future generations' ability to fulfill their needs. A generally accepted concept is that sustainable development involves the balance between environmental, economic, and social aspects (Atilgan and Azapagic, 2016). Since then, sustainable development has increased its importance over the years (Fauzi et al., 2019).

Sustainability has become a key factor in the development of large corporations and cities. It is a fact that sustainable development generates benefits for society as a whole. In this sense, in 2015, the United Nations developed the Sustainable Development Goals (SDGs), comprising 17 goals and 169 targets to integrate issues related to sustainable development in economic, environmental, and general social structures of its signatories (Caiado et al. 2018; Salvia et al., 2019). SDGs are global goals with priorities and aspirations to achieve sustainable development by 2030. The 17 goals comprise several areas, such as poverty; hunger; health education; gender equality; clean water and sanitization; energy; decent work and economic growth; industry, innovation and infrastructure; inequalities; sustainable cities and community; responsible consumption and production; climate action; water and land; justice and institutions; and, partnership. Thus, SDGs demand global action between governments, businesses, and civil society to end poverty and create a life with dignity and opportunities for all (McArthur and Rasmussen, 2018, Leal Filho et al., 2018).

Countless methods have been developed to assess sustainability. In this context, Life Cycle Assessment (LCA) is an important tool for scientific investigations in different areas; it is configured as one of the main methods to translate the science of sustainability into useful knowledge to support commercial and regulatory decision-making (Li, Roskilly and Wang, 2018). LCA is a tool used to evaluate the environmental impacts resources used of a product, service or process considering the life cycle perspective, i.e., from raw material acquisition, production and use phases, to waste management. (Finnveden et al. 2009). LCA is normalized by ISO 14040 (2006), which defines all the steps for its use: goal and scope definition, inventory analysis, impact assessment and interpretation (Pennington et al. 2004). However, the LCA does not cover sustainability as a whole, only the environmental dimension. In this sense, due to the need to carry out a broad and complete approach to sustainability, the Life Cycle Sustainability Assessment (LCSA) was developed (Klöpffer, 2008).

The development of LCSA originated from the need to incorporate the three pillars of sustainable development (environmental, economic, and social impacts) in a single formulation, maintaining the life cycle perspective (Fauzi et al., 2019). Thus, the traditional LCA methodology was expanded in order to understand the economic and social analyses (van Kempen et al., 2017). Unlike traditional sustainability assessment tools, LCSA can identify the sustainability of a product from a life cycle perspective (Ren et al., 2015). According to Klöpffer (2008), LCSA results in LCA integration, Life Cycle Cost (LCC), and Social Life Cycle Analysis (S-LCA). Although LCA is the most popular tool, there are great efforts to develop methodologies for the LCC and S-LCA analyses (Ren et al., 2015).

As a decision support tool, LCSA provides an overview of the sustainability performance of production systems, highlighting areas of significant negative impact, where improvements can be made, or positive impacts where opportunities can be explored (Kabayo et al. 2019). In addition, LCSA can be used in policy recommendations, aiming at improving the sustainability of a given system (Roinioti and Koroneos, 2019), and also as a source of competitive advantage for companies and organizations (Settembre Blundo et al., 2019). Searches of companies, industries, and organizations for a broad sustainability analysis also benefit from a commitment to the SDG (Wang et al., 2018).

One of the top 17 SDGs is ensuring sustainable consumption and production standards. With this growing interest in sustainable products, more studies are introducing the sustainability concept and sustainability assessment tools for strategic decision-making systems in order to improve the sustainability performance of products (Hannouf and Assefa, 2018). To advance towards sustainable development, a more holistic approach to sustainability is required (Ekener et al., 2018). In this context, it is perceived that the application of LCSA has been increasing in recent years. LCSA assists organizations, industries, and countries to achieve their goals with a view to sustainable development and service to the SDG. The broader analysis of the LCSA encompasses all SDGs in its evaluation, and is thus an important tool to help organizations identify the environmental, social, and economic impacts of their activities from a life cycle perspective (Ren et al., 2015; Van Kempen et al., 2017).

This study was developed through a bibliometric and systematic research of the scientific literature of studies on LCSA. A bibliometrics review comprises a quantitative analysis of scientific production on a given topic, elaborating on scientific indexes that translate the main aspects of the publications. The scientific indexes elaborated on by the bibliometric study comprise the temporal analysis of the theme, number of publications, authors, countries of periodical publications, and frequency of keywords, among others. These indexes help us have a greater understanding of the subject studied, promoting an overview of, for example, the main authors, periodicals, and keywords used in the studies, besides contributing to the state-of-the-art analysis of this theme (Visentin et al., 2019a). In this analysis, a Bibliographic Portfolio (BP) is selected according to pre-established criteria, and later the bibliometric analysis of scientific indexes is performed.

On the other hand, the systematic review comprises a qualitative analysis of BP studies. This analysis is deeper and involves, for example, the categorization of articles, thematic analysis, and detailing of methodologies (Visentin et al., 2019a). In addition, this analysis also evidences the highlights and knowledge opportunities found in BP. The results of the bibliometric and systematic research summarize the knowledge of the subject and provide important information about current and future research directions.

Bibliometric and systematic studies have been gaining popularity in recent years, being present in several areas of knowledge, such as LCA and remediation (Visentin et al. 2019), toxicology of nanoscale zero valent iron used in soil remediation (Vanzetto and Thomé, 2019), sustainable remediation (Braun et al., 2019), robotics in surgery (Shen et al., 2019), infrastructure (Ferrer, Thomé and Scavarda, 2018), family business succession (Cisneros et al., 2018), agriculture (De Luca et al., 2017), renewable energies (Azevedo, Santos and Antón, 2019), sustainable development (Caiado et al., 2017), and implementation of the sustainable development goals (Caiado et al. 2018), among others.

This research intends to contribute to the scientific community on the subject studied, since it presents a representative selection of international research in an interdisciplinary area. The new contributions of the present study are: (i) to broaden the literature review, providing scientific indexes; (ii) to map the main sectors and locations of LCSA studies applied; and (iii) to identify the main indicators and methodologies of each dimension of sustainability used in the bibliographical portfolio studies; (iv) listing and detailing the main methodologies employed in the LCSA results' final analysis and (v) presents the main recommendations for future research.

Thus, this article aims to identify and map the LCSA application in the main scientific databases, through a process of bibliometric and systematic literature review.

To this end, some specific objectives were outlined: (i) to select a bibliographic portfolio that addresses the theme of LCSA; (ii) to perform a bibliometric analysis of the selected bibliographic portfolio, developing scientific indexes; (iii) to perform a thematic synthesis; and (iv) to evaluate the main indicators and methodologies used by the articles in the bibliographic portfolio.

2. Methodology

This study is characterized by a systematic and bibliometric research of an exploratory and descriptive nature, with qualitative and quantitative approaches, to locate and analyze existing studies related to LCSA, with an aim to increase the knowledge related to the theme. The methodology of this research is based on Visentin et al. (2019a).

2.1 Delimitations of the Research

For the selection of the BP, some delimitation criteria were considered. The first delimitation considered was the origin of the articles. Only scientific articles published in journals were considered. This type of publication goes through a peer review process, which increases the article quality.

As for the years of publications, there was no delimitation, since the theme of LCSA is relatively new. However, the BP of this research comprises all the articles published until the end of 2019.

The databases surveyed were delimited according to the criteria of the program used for data analysis. The Bibliometrix program operates in the data analysis of the databases Scopus and Web of Science; thus, the research of the articles was carried out only in these two scientific databases. These databases contain the most abstracts and literature citations reviewed by pairs of multidisciplinary fields, as well as bibliometric tools to track, analyze, and visualize surveys.

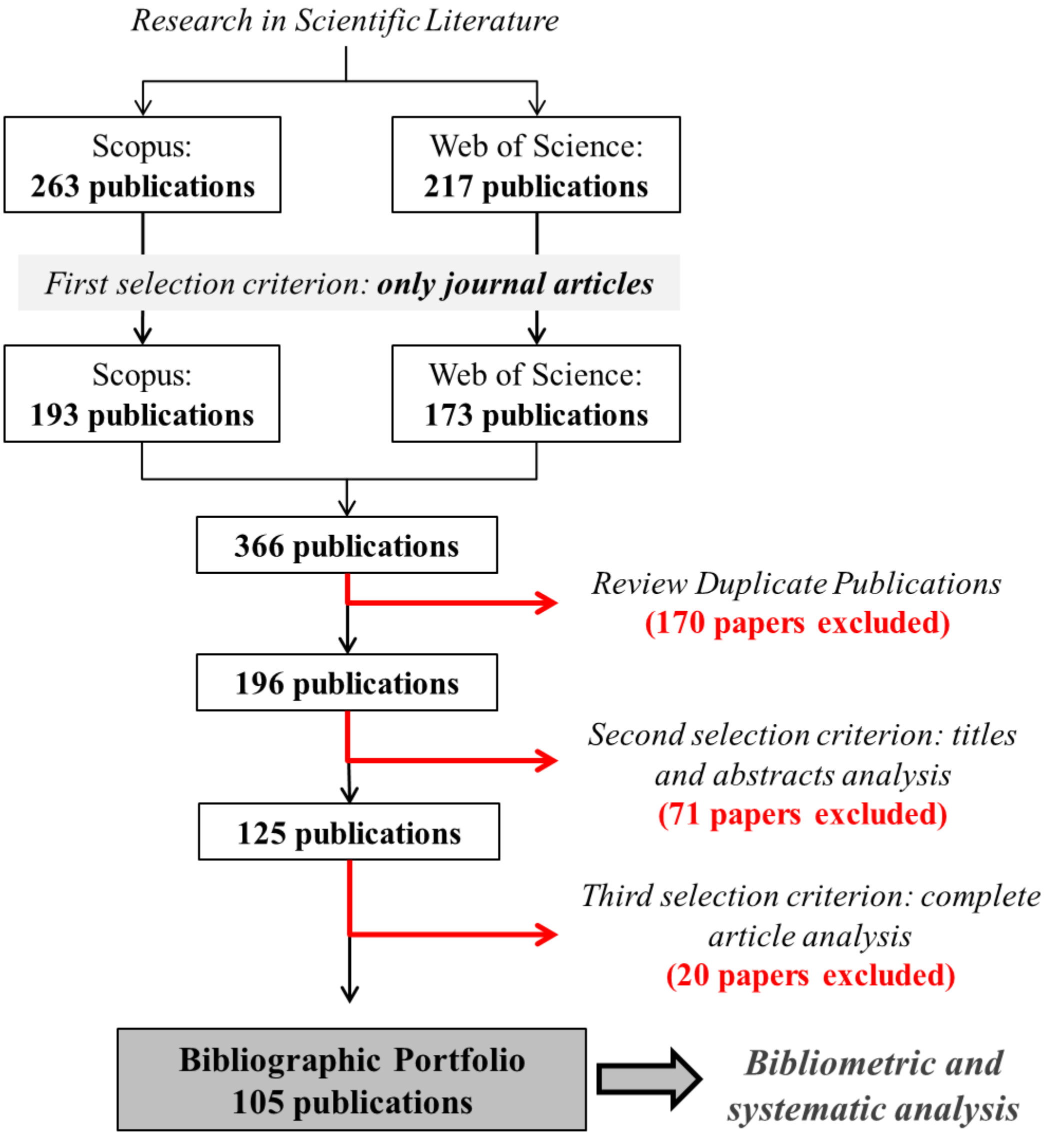
2.2 Procedure for Selecting the Bibliographic Portfolio

BP selection began with the search in the databases through the use of keywords and boolean operators. The combination of keywords and operators was "Life Cycle Sustainability Assessment" OR "Life Cycle Sustainability Analysis" OR "Life Cycle Sustainable Assessment" OR "Life Cycle Sustainable Analysis" OR "LCSA". Variations in writing were used, since these variations can be observed in the studies. The "OR" operator means that the search will contain one term, the other term, or both. The terms' combinations were delimited with titles, abstracts, and keywords of publications.

The initial survey generated 366 publications, including 193 publications in Scopus and 173 in Web of Science (WOS). The selection of items to compose the bibliographical portfolio followed several stages, which were performed according to the method of Caiado et al. (2017) and Visentin et al. (2019a). Figure I - 1 illustrates the process of selecting the BP. The raw data were initially filtered, considering only articles published in journals, after eliminating repeated and redundant papers (170 articles were excluded). Then, the relevance of the articles according to their titles and abstracts was classified (71 non-relevant articles were excluded). The exclusion criteria of the articles used were: (i) not to understand a complete sustainability analysis, considering the environmental, economic, and social aspects (articles that did not evaluate all three aspects were excluded) and (ii) be outside the scope of the LCSA analysis, consisting of another evaluation that does not employ the LCA method. The exclusion criteria were applied in the title and abstract analysis, as well as the complete article analysis. Afterward, an analysis of the complete articles was performed (20 articles were excluded).

Thus, the BP was constituted according to the specified search criteria and the representativeness of the articles in the theme of the LCSA. The BP of this research was composed of 105 articles for this review. All BP articles are presented in the Supplementary Material.

Figure I - 1: Methodological procedures for the bibliographical portfolio selection (based on Visentin et al. (2019a)).



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2.3 Bibliometric and Systematic Analysis

The bibliometric research of the BP final articles was carried out through the Bibliometrix program (Aria and Cuccurullo, 2017). In this program, the data were analyzed based on the publication year, authors, affiliations, journals and impact factors, countries, main thematic areas, the most used keywords, and the co-occurrence network of keywords. In the thematic areas analysis, the studies were categorized according to the thematic areas classification of the Scopus and WOS databases. The data resulting from the program analysis were compiled into a Microsoft Excel spreadsheet for chart and table elaboration. The 10 most frequent keywords were selected, and for the co-occurrence network analysis, 25 more frequent keywords were used to better represent the relationships.

The systematic analysis comprised a content analysis. Initially, a categorization of the BP articles according to the type of study; sectors of studies' applications and localizations; methodologies for each life cycle analysis (LCA, LCC, and S-LCA) used or developed; environmental, economic, and social indicators used in the studies; and the studies' final results.

The types of study were classified as application of existing methodologies and development of methodology and application, review, or others, which would be theoretical discussion articles on LCSA. The application studies were detailed regarding the application sector in electricity and heat production; agriculture, forestry, and other land use; buildings; transportation and automobiles; industry; waste; and other, as well as the location of the study's application for cities, countries, or continents. The economic sectors of classification of the studies were defined based on the classification used by the United States Environmental Protection Agency (USEPA, 2020). The final results of the studies were evaluated as to how these results were presented, with or without data aggregation—that is, if the individual results of each life cycle analysis were evaluated and if some methodology was employed, or if there was aggregation of the results of the analyses in a single sustainability score, and which method was employed.

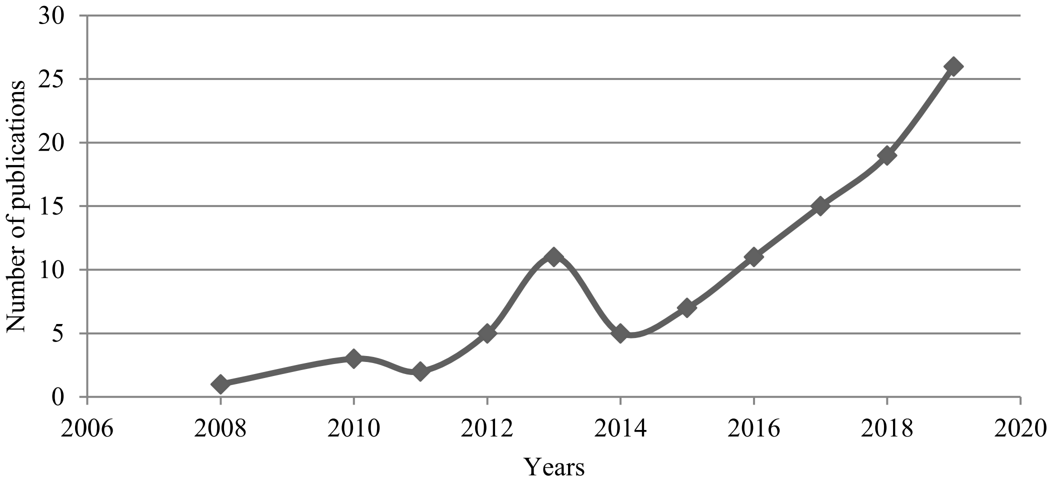
The data resulting from the analysis of the program were compiled into a Microsoft Excel spreadsheet for the elaboration of charts and tables.

3. Results and Discussion

3.1 Evolution of Scientific Production over Time

Figure I - 2 shows the evolution of scientific production in the period 2008 to 2019.

Figure I - 2: Temporal evolution of scientific literature on LCSA.



Source: own elaboration.

The first article was published in 2008, and until 2010, there was an annual average of two articles. A sudden increase occurred from 2012. In 2013, the *Journal of Life Cycle Assessment* opened a call for work related to LCSA, subsequently boosting the number of publications in 2013. Since 2015, the number of published documents has had a continuous and exponential growth, with a peak in 2019, the year with the most documents issued (26 in total). The annual average publication number from 2015 was more than 14 articles.

The observed trend is that the publications in the LCSA area grew over the years. The increase in publications was expected due to the efforts of the scientific community in studies and the development of methods and applications aimed at making LCSA more practical and standardized.

3.2 Journals

The distribution of articles by journals includes 33 different sources, reflecting a wide variety of multidisciplinary sources. Table I - 1 presents the data from journals, as well as the number of citations of each of these sources and their impact factors. In this table are the data of journals with two or more publications, as well as journals with a single publication but a high citation and impact factor.

As noted, the main periodical is specifically related to the area of LCA. The other journals involve several areas, such as energy, waste, construction, environment, and sustainability. The number of publications and the total number of citations were related in most journals, since four of the five main journals in number of articles were equally among the first five in number of citations. In other words, it is perceived that the sources with the greatest number of publications were also those that had the greatest impact in the field of research. It is worth highlighting the work published in the journal *Environmental Science & Technology* obtained the third-largest amount of citations. This work configures the works most cited by the academic community, due to its importance in the LCSA context (Guinee et al. 2011).

Table I - 1: Journal publications, citations, and impact factors.

Journals	**Number of publications**	**Number of citations**	**Impact Factor**
The International Journal of Life Cycle Assessment	25	876	4.868
Sustainability	16	197	2.592
Journal of Cleaner Production	15	412	6.395
Journal of Industrial Ecology	6	134	4.826
Applied Energy	5	69	8.426
Sustainable Production and Consumption	4	32	
Chemical Engineering Transactions	2	5	
Energy	2	70	5.537
Energy Policy	2	100	4.039
Renewable and Sustainable Energy Reviews	2	119	10.556
Waste Management and Research	2	13	2.015
International Journal of Energy Research	2	19	3.343
Environmental Science & Technology	1	170	7.149
Science of The Total Environment	1	29	5.589
International Journal of Hydrogen Energy	1	36	4.084
Ecological Economics	1	59	4.281
Industrial and Engineering Chemistry Research	1	26	3.375

The journal with the highest impact factor is *Renewable and Sustainable Energy Reviews* at 10.556, followed by *Applied Energy* at 8.426 and *Environmental Science & Technology* at 7.149. The impact factors of the five journals with the highest number of publications are: *Applied Energy* at 8.426, *Journal of Cleaner Production* at 6.395, *International Journal of Life Cycle Assessment* at 4.868, *Journal of Industrial Ecology* at

4.826, and *Sustainability* at 2.592. Thus, it is perceived that the impact factor varies from journals that do not yet have this value until 10.556. The impact factor is evaluated annually by Thomson Reuters (JCR) and is considered the main evaluation metric of scientific journals. This metric considers the number of publications in a journal that are cited within a period of one year (Visentin et al. 2019a).

3.3 Authors, Affiliations, and Countries

Table I - 2 presents the 10 main authors of the BP according to the number of publications, its h-index, linked university, research area, and country. These authors are predominantly civil and environmental engineering and chemical engineering, and are located in Europe, North America, and Asia. Some authors have a large h-index, indicating an influential position in the field.

Table I - 2: The BP authors by number of papers, h-index, institution, research area, and country.

Authors	Number of articles	h-index*	University	Research area	Country
Kucukvar, M.	8	30	Qatar University	Civil Engineering	Catar
Onat, N.C	8	18	Qatar University	Transportation Research	Catar
Finkbeiner, M.	8	38	Technische Universität Berlin	Sustainable Engineering	Germany
Ren, J.	7	25	The Hong Kong Polytechnic University	Industrial and Systems Engineering	China
Tatari, O.	6	34	University of Central Florida	Civil and Environmental Engineering	United States
Traverso, M.	6	19	Technische Universität Berlin	Sustainable Engineering	Germany
Azapagic, A.	4	52	The University of Manchester	Chemical Engineering and Analytical Science	United Kingdom
Zamagni, A.	4	14	Italian National Agency for new Technologies, Energy and Sustainable Economic Development)	Civil and Environmental Enginering	Italy

Authors	Number of articles	h-index*	University	Research area	Country
Dong, L.	3	17	University of Alabama	Chemical and Biological Engineering	United States
Halog, A.	3	17	University of Maine	Industrial Ecology	United States
Lehmann, A.	3	10	Technische Universität Berlin	Environmental Technology	Germany
Tarne, P.	3	3	Technische Universität Berlin	Sustainable Engineering	Germany

* h-index source: Google Scholar and Scopus.

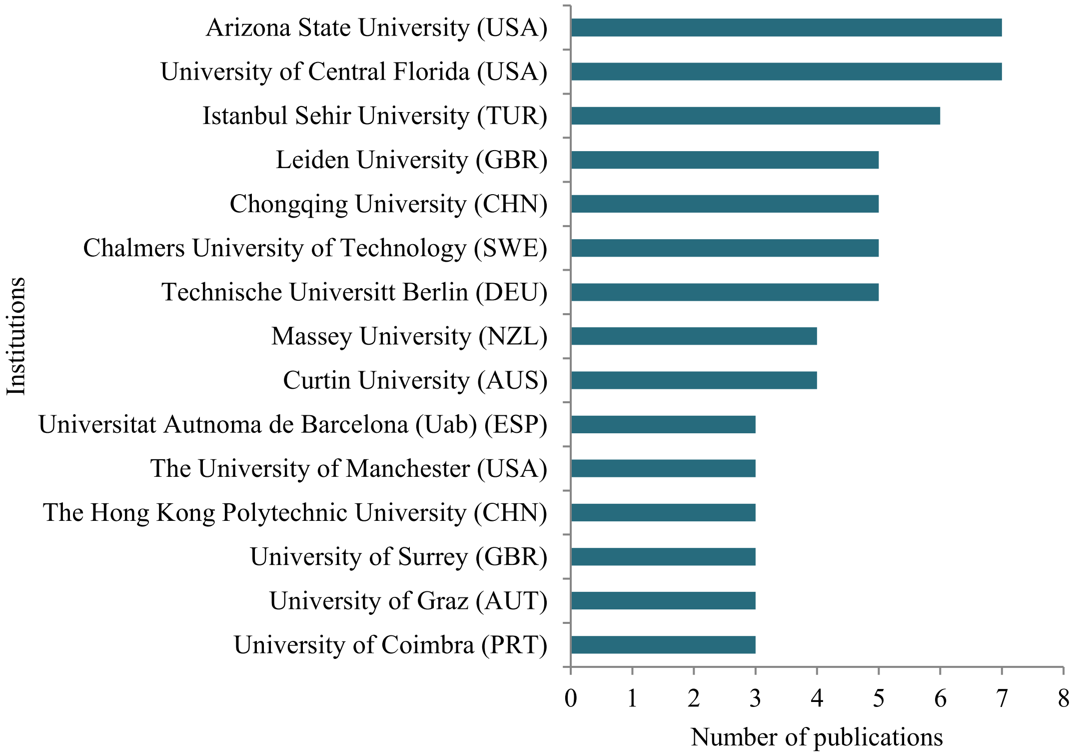
It is worth mentioning that, the authors who have the biggest share as the main author in the BP. In this way, of the top 10 authors, only Nuri C. Onat is the main author in all eight publications. In this sense, main author is described as the paper first author. Jingzheng Ren is the firts author in six publications. Matthias Finkbeiner, Alessandra Zamagni, and Anthony Halog are major authors in one publication. The others authors are mostly co-authors of the BP publications, such as Murat Kucukvar, Omer Tatari, as well as Marzia Traverso, and Liang Dong. Furthermore, of the BP authors only 6 are unique authors, and the author Jingzheng Ren is the only author in two papers.

In Figure I - 3, the main affiliations of the authors of the BP are detailed. The descriptive statistics of the BP demonstrates that the authors affiliated to two American universities namely 'University of Central Florida' and 'Arizona State University' published the highest number of articles. The others affiliations are related to countries like United Kingdom, Germany, Sweden, Turkey, China, Japan, Thailand, Iran, and Qatar.

Furthermore, 39 publications of the total BP articles have a unique affiliation, that is, all authors are of the same affiliation.

It is also noteworthy that most of the major authors are associated with the affiliations most frequently observed in the BP (see Figure 3 and Table 2), whereas some non-major authors are not associated with those affiliations. For example, Matthias Finkbeiner and Marzia Traverso associated with Technische University Berlin and Jingzheng Ren associated with Hong Kong Polytechnic University. However, some of the authors are associated with different institutions of the main affiliations, such as the authors Murat Kucukvar and Nuri C. Onat with Qatar University and Alessandra Zamagni with the Italian National Agency for new technologies, both energy and sustainable economic.

Figure I - 3: Main BP research institutions.



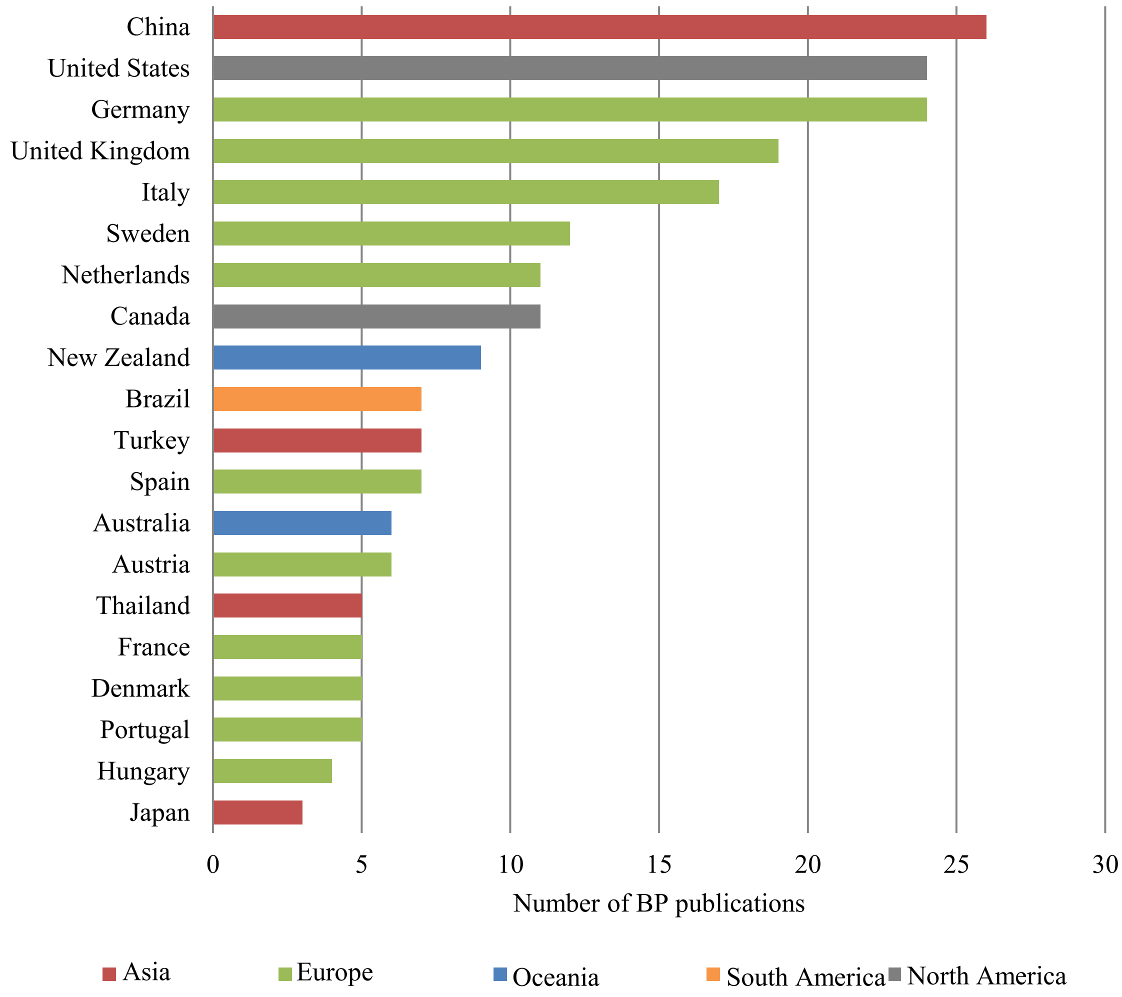
Source: own elaboration.

Figure I - 4 presents the geographic distribution of the main articles that are part of the BP. It is perceived that the vast majority of countries (54%) are European, the main countries being Germany, the United Kingdom, Italy, Sweden, and the Netherlands. While 22% are from Asia and 15% from North America, the presence of Oceania (7%), South America (3%), and Africa is still noteworthy. These percentages were defined through the relationship between the numbers of publications from each country on the continents in relation to the total number of BP publications. This makes it clear that the larger amount of publications are set up in Europe, but there is a good distribution of publications worldwide, demonstrating the global effort to improve studies in the field of LCSA.

Furthermore, 68 publications of the total of BP's articles are from unique countries, that is, all authors are from affiliations from the same country. While, 35% of publications refer to collaboration between authors from different countries.

Another factor that can also be highlighted is that most publications are verified in developed countries. In these countries, the adoption of sustainable practices is already in broad development and application, which also favors the inclusion of sustainability in the broader analysis of the life cycle. The adoption of sustainable practices in developing countries is still at an early stage, with some measures already developed and implemented. However, in this sense, China, which configures as a developing country, has the most publications. There are great political and scientific efforts in search of more sustainable practices of production, consumption, and even contaminated site remediation (Visentin et al. 2019a).

Figure I - 4: Main countries in terms of scientific production on LCSA.



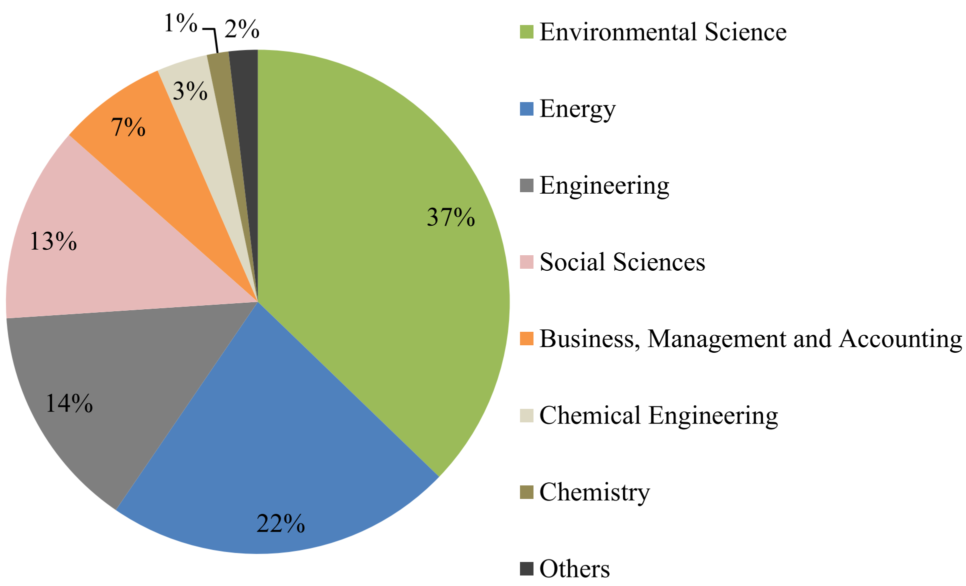
Source: own elaboration.

The main authors of the BP are of different affiliations (Table I - 2), and these are generally related to the main countries of the publications. Eight of the top 10 authors relate to the top five countries of the publications (Germany, the United States, the UK, China, and Italy). Those that escape from this panorama are the authors from Asia, Murat Kucukvar and Nuri C. Onat.

3.4 Thematic Areas

In relation to thematic areas, the publications on LCSA come from a multidisciplinary approach, as shown in Figure I - 5. Most publications are from the area of environmental sciences (37%); followed by energy (22%); engineering (14%); social sciences (13%); and business, management, and accounting (7%). In addition, other thematic areas are also observed, such as chemical engineering (3%), chemistry (1%), and others (e.g., economics, econometrics and finance, physics and astronomy, biochemistry, and genetics and molecular biology (2%)). The percentages were defined based on the number of publications from each thematic area in relation to the total of BP articles.

Figure I - 5: Main thematic areas of the bibliographic portfolio.



Source: own elaboration.

3.5 Keyword Analysis

Keywords represent the basic units of a specific field of study and can provide a view of knowledge structures and search trends. Two analyses of keywords were performed, the first referring to the frequency of keywords used and the second of keyword co-occurrence. This analysis of co-occurrence maps a network of words, where each node represents a keyword and the link between the nodes represents the co-occurrence of the keywords (Azevedo, Santos, & Antón, 2019).

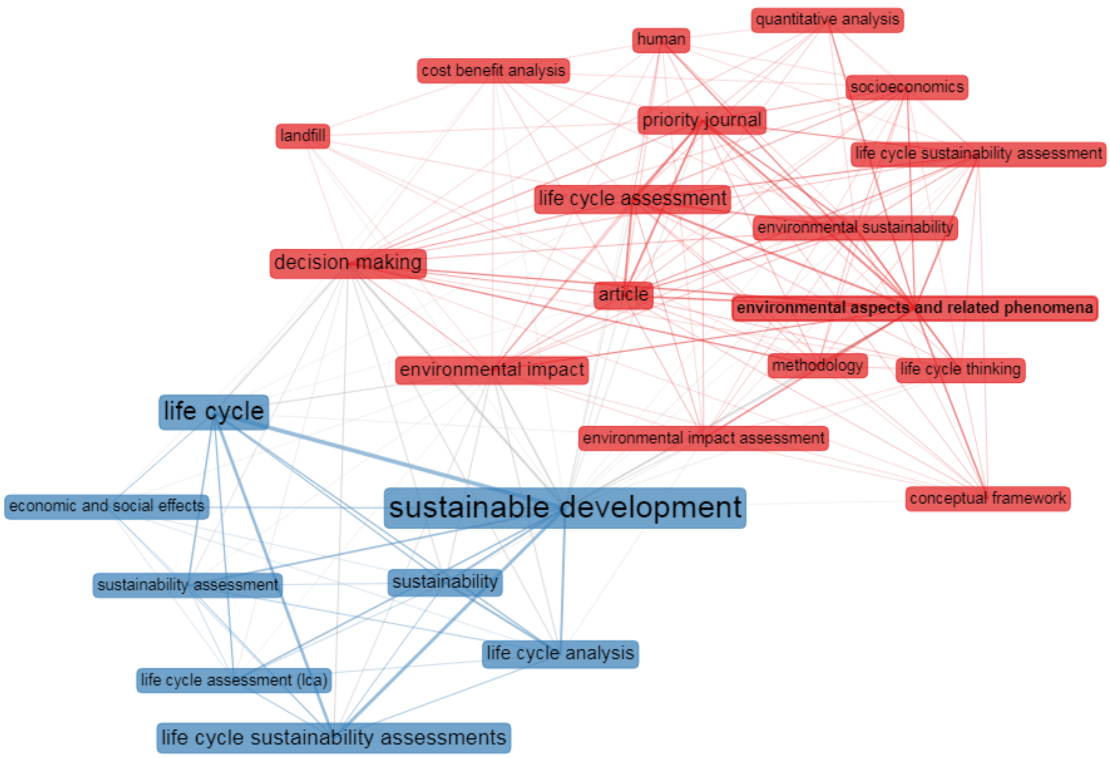
The 10 most prominent keywords in BP studies are *sustainable development* (59 occurrences), *life cycle* (45), *decision making* (36), *life cycle sustainability assessments* (33), *life cycle analysis* (29), *sustainability* (26), *environmental impact* (25), *life cycle assessment* (23), *sustainability assessment* (18), and *environmental sustainability* (15). This analysis highlights that the literature on LCSA is linked to sustainable development, life cycle analysis, decision-making, and sustainability. However, among the dimensions of sustainability, the environment stands out in this issue.

Figure I - 6 presents the keyword mapping, with a minimum limit of 25 keywords and nodes to provide a deeper analysis of the literature characteristics. This mapping was performed by Bibliometrix. Each keyword expressed corresponds to a node in the network, and the occurrences of the keywords constitute the edges between the nodes. In a sentence, if two keywords have a co-occurrence relationship, this means that there is a connection between the two nodes in n-order (Azevedo, Santos, & Antón, 2019).

The application of this methodology identified two main clusters. The smallest (blue) cluster is concerned with sustainable development and LCA, covering concerns with life cycle sustainable analysis, sustainability, sustainability analysis, and economic and social effects. The red cluster presents the keywords related to the life cycle sustainability analysis, environmental aspects, and decision-making. In this cluster, we perceive the predominance of environmental aspects, but it is verified that economic and social aspects, represented by cost-benefit analysis and socioeconomic and human values, are included. In this cluster, there are also aspects of methodologies, frameworks, and quantitative analysis, demonstrating that many of the BP studies were based on the development of methodologies.

The blue cluster is heavily connected to the red cluster, since there are many connections between them. The main link between clusters is decision-making. This aspect is linked to all keywords, since decision-making is one of the main contributions of LCSA, assisting decisions, organizations, and industries in search of a greater knowledge of the environmental, economic, and social impacts of products and processes, aiming at sustainable development.

Figure I - 6: Keyword co-occurrence network.

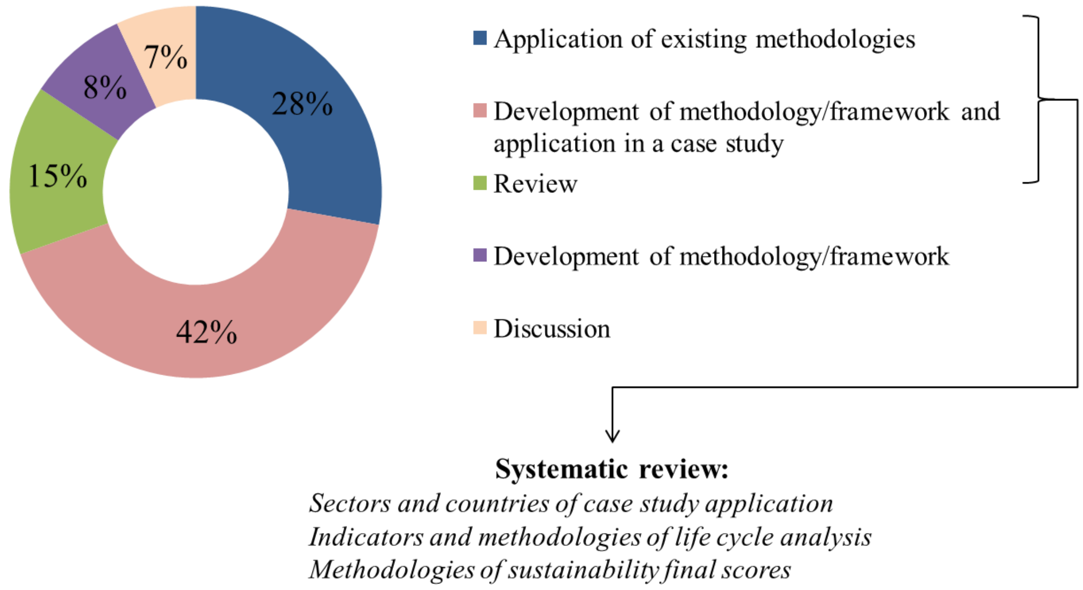


Source: own elaboration.

3.6 Systematic Review

The articles that compose the BP were categorized according to the type of study (application, development of methodologies, review, or others), detailing the areas of application of the applied studies, as well as the location when it was informed by the authors, and also in relation to the final data of the studies applied, demonstrating whether there was aggregation of the LCA results, and in these cases, which method was employed. Figure I - 7 shows the type of BP study. The predominant type of study in the BP is application, corresponding to 70% of the studies. These percentages were determined through the relationship between the types of studies and the total of BP publications.

Figure I - 7: Quantitative distribution of type of BP studies.



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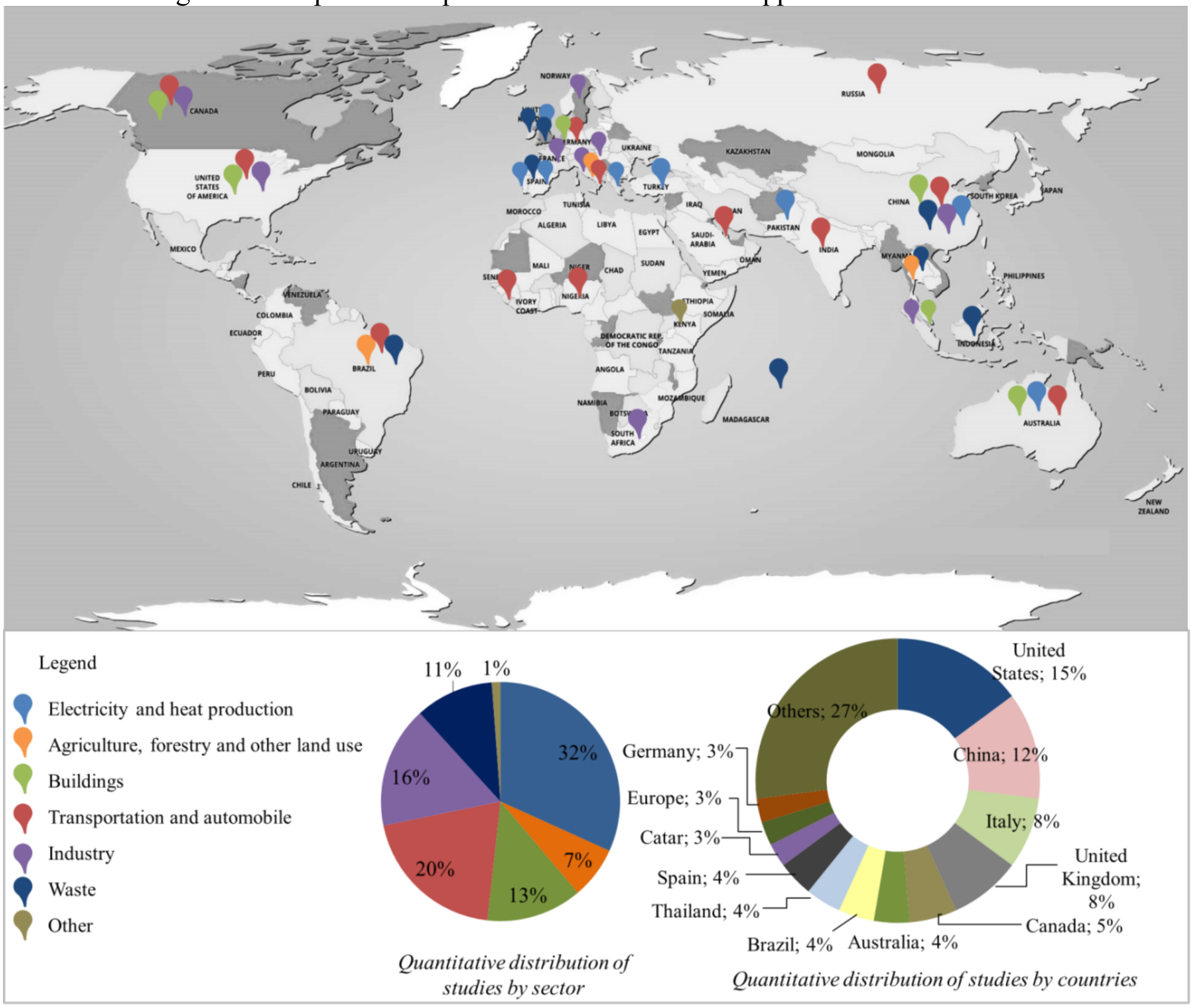
3.6.1 Sectors and Countries of Case Study Application

Figure I - 8 illustrates the spatial and quantitative distribution of the application studies according to sector and country of localization, when it was indicated by the authors. The application studies were classified as to the sector that it was applied in: electricity and heat production; agriculture, forestry, and other land use; buildings, transportation, and automobiles; industry; waste; and others (USEPA, 2020). The industrial sector is formed by manufacturing industries of chemicals; wood, wood products and furniture; machinery and equipment, and non-metallic minerals. The map illustrates through markings the localities where the studies occurred and which sectors were studied, but not the quantity of studies or applications. The quantitative analysis of the distribution of the studies is represented in the charts below the map.

Figure I - 8: Spatial and quantitative distribution of applied BP studies.



Source: own elaboration.

In the localization analysis, the distribution of studies encompasses four continents. The majority of the studies, in relation to quantity, concentrate on European (38%), followed by Asia (27%), North America (20%), and South America (7%). There are also studies from Africa (4%) and Oceania (4%). The distribution in the countries illustrates that the largest number of studies were applied in the United States (15%), China (12%), Italy and the United Kingdom (9%), and Canada (6%). The other countries that were localities of studies were Greece, Holland, Hungary, Mauritius, India, Indonesia, England, Ireland, Malaysia, Nigeria, Pakistan, Portugal, Kenya, Russia, Sierra Leone, Sweden, Turkey, Singapore, and South Africa. All the percentages presented above were determined through the relationship between the articles of each country and continents with the total number of application studies.

Most of the studies were applied in the electricity and heat production sector (32%), followed by the transportation and automobiles sector (20%) and industry (16%). The other sectors were buildings (13%); waste (11%); agriculture, forestry, and other land use (7%); and others with a focus on communitarian services (1%). These percentages were defined based on the number of articles in each sector in relation to the total number of application studies. A relationship can be established between the most studied sectors and the authors who published the most in the BP. For example, Jingzheng Ren published 22% of the energy sector studies, while Murat Kucukvar and Nuri C. Onat added 35% of the publications in the transport and automobile sector. The categorization of articles by sector can be checked in detail in the Supplementary Material.

The electricity and heat production sector is the most studied in BP studies. All sectors and production processes, as well as the general population, require direct or indirect energy for their implementation. Thus, the study of life cycle sustainability in this sector is important to evaluate the impacts associated with energy sources, assisting in a decision-making aimed at sustainability. BP studies vary in application as compared to the impacts of various energy sources (Halog and Manik, 2011, Stamford to Azapagic, 2012; Stamford and Azapagic, 2014; Pesonen and Horn, 2013; Ren et al., 2015; Yu and Halog, 2015; Atilgan and Azapagic, 2016, Huang and Mauerhofer, 2016, Akber, Thaheem and Arshad, 2017; Ren et al., 2017; Kouloumpis and Azapagic, 2018; Ren, 2018a; Ren, 2018b, Ren et al., 2018; Kabayo et al., 2019; Moslehi and Reddy, 2019; Roinioti and Koroneos, 2019), as well as the evaluation of the sustainability of solar energy (Traverso et al., 2012a.; Li, Roskilly and Wang, 2018; Gwerder et al., 2019), biogas production (Jin et al., 2017), hydrogen production (Ren and Toniolo, 2018; Valente, Iribarren and Dufour, 2019), biorefineries (Keller, Rettenmaier and Reinhardt, 2015), biofuels (Collotta et al., 2019), hydro energy (Guo et al. 2019), and household energy needs (Gwerder et al., 2019).

The transport sector corresponds to 25% of global carbon dioxide emissions (WHO, 2018). The global target of emission reduction defined by the Paris Agreement results in the need for studies in this area. In this sense, the transport sector and vehicles are widely studied by the authors of the BP. These studies involve the production of alternative fuels for transport, such as oxymethylene ether (Mahbub et al., 2019), biomass (Ekener et al., 2018), alternative fuels (Hoque et al., 2019), production of hydrogen from biomass (Stefanova et al., 2014), technological alternatives of vehicles such as electric and hybrid vehicles (Onat, Kucukvar and Tatari, 2014a; Onat, Kucukvar and Tatari, 2016; Onat et al., 2016a; Onat et al., 2016b; Onat et al., 2016c; Onat et al., 2019), car changer (Schau, Traverso and Finkbeiner, 2012), pavement production (Hamdar, Chehab and Srour, 2016; Zheng et al.,2019), battery/electric vehicles, and management of sustainability in automotive companies (Tarne, Traverso and Finkbeiner, 2017; Tarne, Lehmann and Finkbeiner, 2019; Tarne et al., 2019).

The buildings and industrial sector are two of the sectors that most contribute to economic and social growth, corresponding to more than 25% of the world's GDP and the generation of millions of jobs worldwide (Word Bank, 2017). It is acknowledged that the industrial sector and the construction industry are responsible for considerable environmental impacts, so it is important that alternatives to reduce these impacts are explored (Wang et al., 2017; Aldieri, Kotsemir and Vinci, 2019). To this end, the application of LCSA in these sectors seeks to evaluate the associated impacts, in order to improve decision-making and the sector in search of a more sustainable alternative, minimizing the negative environmental and economic aspects and benefiting the positive impacts.

In buildings sector, the BP studies are applied in general construction studies (Ostermeyer, Wallbaum and Reuter, 2013; Onat, Kucukvar and Tatari, 2014b; Hossaini et al., 2015; Dong and Ng, 2016; Gencturk, Hossain and Lahourpour, 2016; Wu et al., 2017; Janjua et al., 2019), concrete recycling studies (Hu et al., 2013), production of concrete structures (Wang et al., 2017), and production of timber for construction (Balasbaneh, Marsono and Khaleghi, 2018).

The application of LCSA in the industrial sector studies in BP is varied and involves several productive processes, such as ceramic production (Traverso et al., 2012b; Ferrari et al., 2019; Settembre Blundo et al, 2019), production of high density Polyethylene (PEAD) (Hannouf and Assefa, 2017; Hannouf and Assefa, 2018), additive manufacturing (Ma et al., 2018), marble production (Valdivia et al., 2013), solvent recovery (Zajáros et al., 2018), production of biological-based products (Martin et al., 2018), production of wood-plastic products (Kua, 2017), production of magnets for wind turbines (Wulf et al., 2017), productive process of sugarcane biorefinery (Nieder-Heitmann, Haigh and Görgens, 2019), macroalgae biorefinery systems (Sadhukhan et al., 2019), and also the production of chemical products (Xu et al., 2017).

The application of LCSA in waste sector covers different ways of waste management, such as municipal waste (Menikpura, Gheewala and Bonnet, 2012; Souza et al., 2015; Wang et al., 2018), recycling of bottom ash (Sou, Chu and Chiueh., 2016), recycling of cooking oil (Vinyes et al., 2013), anaerobic digestion of source-separated food waste (Iacovidou et al., 2017), disposal scenarios for used polyethylene terephthalate (PET) bottles (Foolmaun and Ramjeawon, 2013), agricultural and agroindustrial waste management (Aziz, Chevakidagarn and Danteravanich, 2016), and urban water reuse at various centralization scales (Opher, Friedler and Shapira, 2019). In 2016, the amount of waste generated in the world exceeded 2.01 billion tons. It is estimated that more than 3.5 billion tons of waste will be generated by 2050 (Kaza et al., 2018). In addition, it is estimated that 1.6 billion tons of carbon dioxide emission equivalent were generated from the treatment and disposal of waste in 2016, representing about 5% of the total global emissions (Kaza et al., 2018). This makes it necessary to seek more sustainable waste management alternatives.

Agriculture and food production have been studied by the scientific community of LCSA. It is estimated that, by 2050, the world population will reach more than nine billion (United Nations, 2019). To meet the population demand, it is necessary to increase food production by 70%. Thus, the sustainable management of agricultural and food production is fundamental to sustaining the global population. The LCSA studies in this sector involve the production of soybeans (Zortea, Maciel and Passuello, 2018), cultivation of olives (De Lucca et al., 2018), dairy production (Chen and Holden, 2018), production of animals for consumption (Scherer et al., 2018), use of soil and forests in mangrove management in Thailand (Moriizumi, Matsui and Hondo, 2010), and alternatives for forest preservation (Pizzirani et al., 2018).

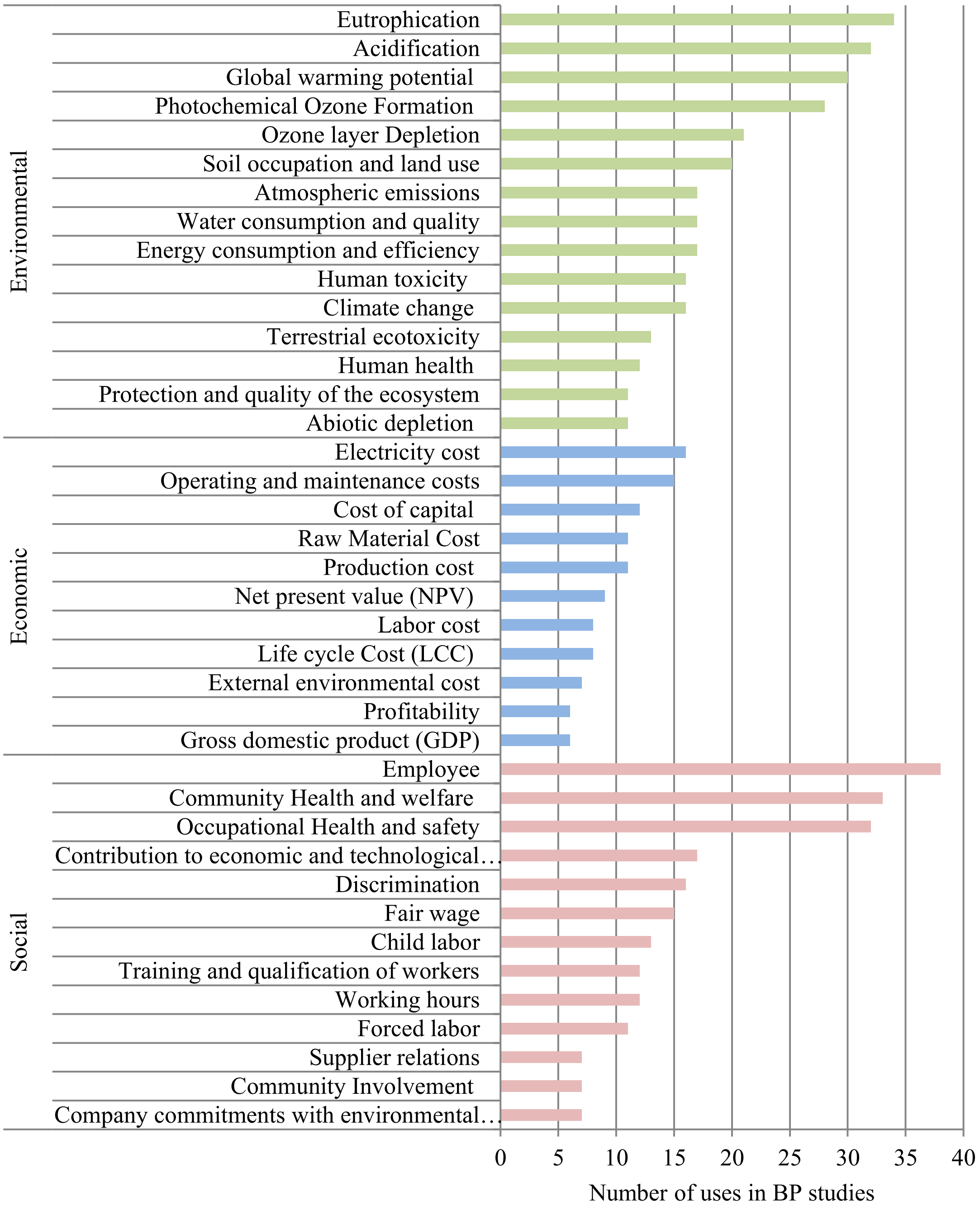
Another study that does not fit in the previously detailed sectors is that of van Kempen et al. (2017), illustrating the application of LCSA in assessing the sustainability of the UN's humanitarian supply chains. The authors verified the impacts associated with the distribution of a set of cuisine provided by a UN agency to the population of Kenya. The expected increase of the world population also threatens to increase economic and social inequality. The application of LCSA in this sense aims to evaluate in a holistic way the best strategies for supplying community aid items, assisting community organizations to determine the most sustainable solutions (Van Kempen et al., 2017).

In the BP studies, the geographical location (i.e, countries, and cities) of the data selected in the analysis can influence the environmental impacts of the study. This fact can be observed, for example, in environmental analyses involving the use of electricity. The production of electricity results in environmental impacts, and this, depending on the source, can increase or decrease the impacts of the studies. In addition, these sources can also influence lifecycle costs and social impacts. For example, Visentin et al. (2019b) noted that countries whose energy matrices are based on renewable sources result in a decrease of more than 70% in total environmental impacts, while in countries where the energy matrix uses non-renewable energy, there are greater associated environmental impacts. Moreover, the costs may vary according to location. Even more social impacts are often dependent on data at the national level, and in this case, are influenced by the social and economic situation of the country in question.

3.6.2 Indicators and Methodologies of Life Cycle Analysis

The main environmental, economic, and social indicators used in BP studies are presented in Figure I - 9.

Figure I - 9: Environmental, economic, and social indicators most used in BP studies.



Source: own elaboration.

The most used environmental indicators in the impact evaluations are eutrophication and acidification, followed by the potential indicators of global warming and the formation of a photochemical ozone. The most used indicators are variable and encompass several environmental segments, such as impacts to air, water, soil, ecosystems, and human beings. Air impacts can be evaluated by indicators such as global warming potential, photochemical ozone formation, ozone layer depletion, atmospheric emissions, and climate change. Many of these indicators are also used to assess human health impacts. The quality of the water and ecosystems is one of the most evaluated factors with the indicators of eutrophication, acidification, land use and occupation, water consumption and quality, energy consumption and efficiency, terrestrial ecotoxicity, ecosystem quality, and abiotic depletion.

Unlike the environmental dimension indicators, which consider complex environmental mechanisms, the indicators in the social and economic dimension are, in most cases, direct (Wang et al., 2018). The necessary data are often information about production and the actors involved. In the economic area, the main indicators used are electricity costs, operating and maintenance costs, raw material, and production and capital costs. In the social area, the main indicators relate to workers, such as employment, welfare of workers and the community, fair salary, discrimination, working hours, number of accidents at work, training, child labor, and forced labor. In many impact assessments in the social area, only the employment indicator was used, not covering all the possible impacts that a given activity can generate.

Unlike environmental analysis, in which there is a greater consensus in the determination of indicators, the economic and social analyses still lack a set of commonly accepted indicators. In the economic issue, many studies encompass direct production costs, such as raw material, energy, and water consumption, not considering, for example, the net present value or gross domestic product, or some studies consider the environmental costs associated with the environmental impacts of the company, such as atmospheric emissions, and others do not. On the other hand, in the social analysis, the main indicator used is employment, and in many analyses, this is the only indicator considered. In addition, in many analyses, only a limited number of social aspects are considered (Ekener et al., 2018). Thus, although there are numerous studies on social and economic indicators, difficulties exist in the lack of a clear process of selecting these indicators (Neugebauer et al., 2015).

The selection of indicators for life cycle analyses, mainly LCA, are concentrated in a limited and recurrent set of indicators, usually available in the analysis methods used (Martin et al., 2018). The selection of indicators should consider the importance of this indicator in the analysis to be performed. Another way to select indicators is by using stakeholders. In the usual analyses of the LCSA, the choice of impact categories is usually made by the analysts themselves, instead of deriving them from the perspectives of the involved stakeholders (Souza et al., 2015). Also, one way to assist in the choice of LCSA indicators is to relate the indicators to the SDGs (Wang et al., 2018). The SDGs aim to advance society toward sustainable development, which should be considered holistically, rather than considering separate environmental, economic, and social impacts. In this sense, the SDG structure can be used as a guide to identify indicators due to their holistic sustainability perspective (Wang et al., 2018). For example, indicators of global warming potential and photochemical ozone formation are directly related to SDGs 3, 9, 12, 13, and 15 (health and welfare, industry, innovation and infrastructure, responsible consumption and production, action against global climate change, and earth life, respectively). Society and human industries are responsible for a large part of atmospheric emissions (SDGs 9, 12, and 13). On the other hand, industries are major contributors to the economy (SDG 8).

Another challenge faced by economic and social analyses is the lack of available databases. Differently from what occurs in environmental data, where there are numerous updated databases that encompass various sectors, products, and locations (e.g., GaBi and ecoinvent), the economic and social databases still need to advance in this direction. For example, the economic database for LCC is still under development, being more advanced in the construction sector, yet some costs are partially included in LCA databases (e.g., GaBi) or displayed by systems management accounting (Neugebauer et al., 2015). On the other hand, social data are difficult to collect. Existing databases are only available in a country or sector, such as the social hotspot Database (Neugebauer et al., 2015).

The LCA, LCC, and S-LCA analyses do not have the same level of maturity, hindering the wide implementation of LCSA (Grubert, 2017). LCA is a method standardized by ISO 14044 (2006) and is widely used to investigate the potential environmental impacts of products and processes (Li, Roskilly and Wang, 2018). LCC is not yet standardized, although it is older than LCA and has been used since the 1930s (Hannouf, and Assefa, 2017). LCC considers all of the costs associated with the life cycle of a product that are directly covered by any actor in the product life cycle (such as supplier, manufacturer, user, or consumer), and externalities can be included (Hunkeler, Lichtenvort and Rebitzer, 2008). S-LCA is not yet a well-developed and standardized methodology. S-LCA evaluates the potential social impacts of products, relating to the different groups of stakeholders affected, such as workers, society, local communities, and consumers (Benoit and Mazijn, 2009). Therefore, due to the lack of standardized methods for the LCC and S-LCA analyses, greater variations of the methods used in these analyses were perceived in the BP studies.

The environmental impacts analysis of BP studies is done essentially with methods of the traditional LCA according to ISO 14040. In these, LCA analyses are performed using computational tools such as SimaPro® and GaBi. Another method used in the studies was the TBL-LCA model (Onat et al., 2016b; Onat et al., 2016c). The TBL-LCA model is an economic input-output (EIO) model developed at the University of Central Florida. This model considers monetary transactions between the sectors that form the economy of the United States, being able to evaluate all the direct and indirect environmental and socioeconomic impacts, considering the supply chain (Onat et al., 2016b; Onat et al., 2016c).

The economic impact analysis is performed mostly by LCC methods. These methods end up varying with each study due mainly to the indicators selected for the analysis and the method of calculating costs. The application of the LCC is made through calculations of estimates of life cycle costs (Roinioti and Koroneos, 2019). For example, for the energy sector, Moslehi and Reddy (2019) developed a method to estimate the life cycle costs of energy analysis, denominated as Energy Cost Intensity (EnCI). This method is the sum of the annualized initial costs of all cost components of a power system, such as annual consumption, operating, and maintenance costs. This method is normalized by unit of area, building, or installation served by the energy system. Another method employed in calculating life cycle costs was the TBL-LCA model (Onat et al., 2016b; Onat et al., 2016c).

The social impacts analysis is also done by life cycle methods such as S-LCA. However, each BP study proposed a different method for analyzing social impacts. As the S-LCA is still in the process of developing methods and case studies, there is still no standardized or widely accepted model to evaluate impacts. In addition, in many studies, the social dimension is considered to a lesser degree in sustainability assessments, though it is included in many cases (Ekener et al., 2018).

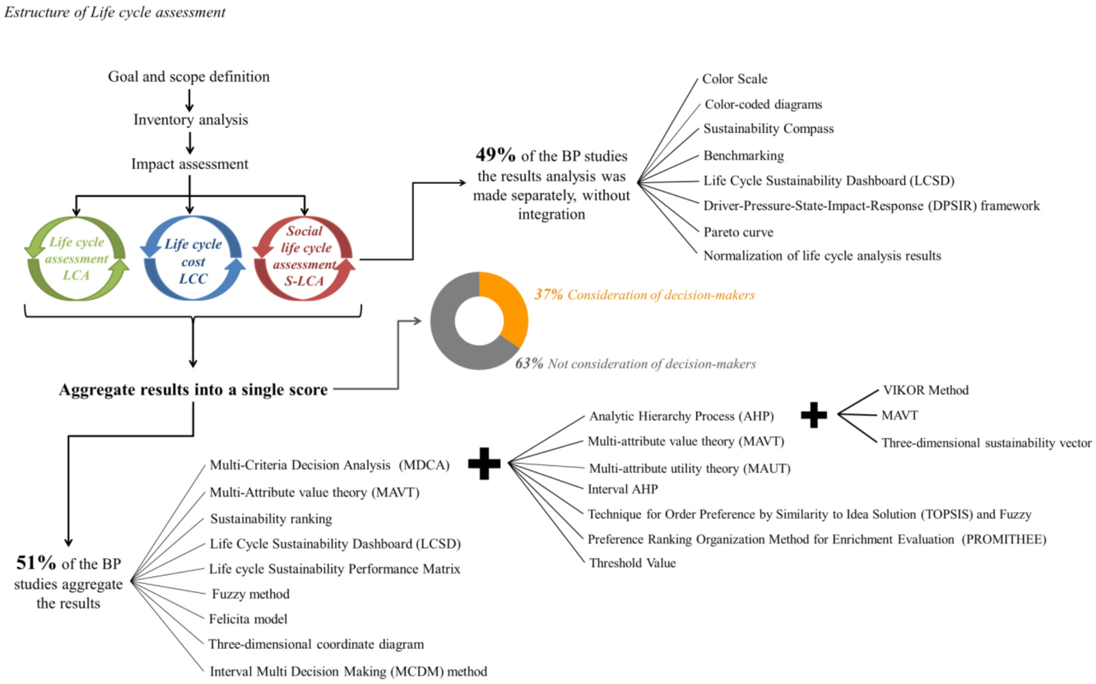
The evaluation of the social impacts of the life cycle in BP studies was done both quantitatively and qualitatively. A method used in the qualitative analysis of social impacts was through the use of a nine-color scale (Yu and Halog, 2015). Most methods employ standardized scores to assess the social impacts of each indicator separately quantitatively (Hannouf and Assefa, 2017; Zajáros et al., 2018; Hoque et al., 2019), as well as semi-qualitative scores (Wang et al., 2018). Also, in some studies, the normalized scores are used in an aggregation calculation to determine a single social life cycle score (Akber, Thaheem and Arshad, 2017; Ekener et al., 2018; Li, Roskilly and Wang, 2018; Janjua et al., 2019; Roinioti and Koroneos, 2019). Other methods employed were the method of the authors Ciroth and Franze (2011) (Van Kempen et al., 2017), and the Life Cycle Sustainability Dashboard (LCSD) (Zortea, Maciel and Passuello, 2018). Settembre Blundo et al. (2019) developed a methodology to analyze at different levels scenarios and perspectives of social impacts (business, workers, and public institutions).

3.6.3 Methodologies of Sustainability Final Scores

The LCSA theorized by Klöpffer (2008) illustrates a combination of three life cycle approaches—environmental, economic, and social—through the relationship LCSA = LCA + LCC + S-LCA. The sum sign of the relationship represents an integration of the three tools (LCA, LCC, and SLCA) in the LCSA, in order to identify the sustainability of a life cycle perspective, analyzing and identifying the performances of a product/process from the environmental, economic, and social aspects (Ren et al., 2015). Numerous methodologies for evaluating LCSA have been developed over the years.

In practice, two LCSA approaches are observed in the studies. The first considers the life cycle analyses results evaluation (LCA, LCC, and S-LCA) separately, concluding the fence of sustainability in a comparative way. The second approach considers the results aggregation of the three life cycle analyses into a single life cycle sustainability score. The first approach is usually more qualitative, while the aggregation of results is quantitative. In BP studies, 51% of the studies performed aggregation of the results of the life cycle analyses in a single score. Figure I - 10 presents the structure of the life cycle analysis and the main methodologies observed in the BP studies to aggregate the results in a single score, and also in the analysis of these in a separate way.

Figure I - 10: Structure of life cycle assessment and main sustainability analysis methodologies used in BP studies.



Source: own elaboration.

LCSA applications, in many cases, lack a final stage of integration for the different perspectives of sustainability. This omission requires users to make an integrated consideration of the sustainability global impact without any methodological support (Ekener et al., 2018). Many of the BP studies present the LCSA results in a separate way, comparing the results; however, some use methodologies for this analysis, such as a color scale and color-coded diagrams, which classify environmental, economic, and social impacts according to magnitude (Corona and San Miguel, 2019; Kabayo et al., 2019). This type of approach assists in the impact visualization, improving the sustainability analysis. Another methodology employed was the Sustainability Compass (Moslehi and Reddy, 2019), which consists of the graphical representation of the results of the life cycle analyses. In addition, comparative benchmarking analyses were also used (Keller, Rettenmaier and Reinhardt, 2015; Valente, Iribarren and Dufour, 2019). The methodology of the Life Cycle Sustainability Dashboard (LCSD) was also employed, but without the aggregation stage, only using the analysis through the color scale charts (Valdivia et al., 2013; Zortea, Maciel and Passuello, 2018). The LCSD was one of the first methodologies developed for LCSA. This method consists of an analysis program that separately evaluates each aspect of sustainability through graphic representation on a color scale and also a normalized score according to the method scale. The results can also be aggregated into a single score, a general index, represented by the position of the arrow at the top of the panel (Traverso et al. 2012a).

Another way of analyzing the results was using the Driver-Pressure-State-Impact-Response (DPSIR) framework (Hannouf and Assefa, 2017). This model consists of a systematic structuring of the relations of cause and effect in connection with environmental problems, assisting in the overview of impacts, connecting their origin to the results and developing efficient responses (Hannouf and Assefa, 2017). Another graphic analysis was performed in the study by Ostermeyer, Wallbaum, and Reuter (2013), in which the results are presented in Pareto curve plots, demonstrating the relationship between each sphere of sustainability, verifying areas that need improvement.

Many of the studies perform a normalization of the LCA results through a normalized numerical scale, such as 0.00 to 1.00, in order to provide a better way to compare the results, since these are all on the same scale. This type of methodology was used in the studies by Vinyes et al. (2013) and Onat et al. (2016c). Vinyes et al (2013) used the contribution percentage of each impact to determine the normalized scores. The results' normalization is configured in an initial step in view of the data aggregation in a single life cycle sustainability score.

The BP case studies that performed the results aggregation in a single score most often employed multi-criteria methods (70%). LCSA offers results for the three dimensions of sustainability and can consist of several indicators, so a decision based on the LCSA results in a question of multi-criteria decision, or at least a question of multi-criteria interpretation (Tarne, Lehmann & Finkbeiner, 2019).

The multi-criteria decision analysis (MDCA) methodology encompasses numerous techniques of a simple or combined nature and can be applied in conjunction with other approaches, as verified in most studies. Multi-criteria techniques can be divided into different groups: (i) theory of multi-attribute value, (ii) prioritization and classification methods, and (iii) interactive methods.

In the Multi-Attribute Value Theory (MAVT), decision-makers make a trade-off between alternatives after comparing them to indicators returning a score for each one; the one that obtains the highest score is chosen (Guarnieri et al., 2015). Examples of methods in this category are the Analytic Hierarchy Process (AHP), Simple Multi-Attribute Rating Technique (SMART), and Technique for Order Preference by Similarity to Ideal Solution (TOPSIS). The prioritization methods and classification aim to represent the preferences of decision-makers through binary relations, evaluating the superiority of an alternative in relation to the other (Zabeo et al., 2011). The main methods of this analysis are Electre (elimination and choice expressing reality), Promethee (preference ranking organization method for enrichment evaluation), and VIKOR (multi-criteria optimization and compromise solution). Finally, the interactive methods make it possible to find the dominance of an alternative when positioned against all the established objectives (Guarnieri et al., 2015). Methods such as STEM (the Step Method), Interval Criterion Weights (ICW), PARETO RACE, and TRIMAP (method of learning in linear programming tri-criteria) belong to this category.

The multi-criteria methods associated with other methods are the most common form of use in BP studies. The MDCA with the AHP method is used in 18% of the studies (Hossaini et al., 2015; Grubert, 2017; Iacovidou et al., 2017; De Lucca et al., 2018; Opher, Friedler and Shapira, 2019), while this configuration is also associated with the VIKOR method (6%) (Ren et al., 2015; Zheng et al., 2019) and the Multiattribute method in 3% (Foolmaun and Ramjeawon, 2013). The MDCA and AHP methods were also associated with the three-dimensional sustainability vector (3%) (Xu et al., 2017). A new approach of the AHP method associated with the MDCA was developed, employing interval-scale data to evaluate the method by the agents involved, rather than the normally used scale (Ren et al., 2018). Another association of the MDCA is with the multi-attribute method, present in 15% of the studies (Atilgan and Azapagic, 2016; Aziz, Chevakidagarn and Danteravanich, 2016; Chen and Holden, 2018; Ekener et al. 2018; Roinioti and Koroneos, 2019) and with the Multi-Attribute Utility Theory (MAUT) (Nieder-Heitmann, Haigh and Görgens, 2019). While only the application of the multi-attribute method is verified in 9% of the studies (Akber, Thaheem and Arshad, 2017; Wulf et al., 2017), the multi-attribute method is nothing more than a weighted sum that considers the values of impacts with a weighting factor, obtained as a result of the application of MDCA methods.

The AHP method performs a comparison in pairs of each criterion, establishing a preference classification. This method is relatively simple to use when there are no large quantities of alternatives to be evaluated. In studies involving a large number of criteria, the method ultimately results in many factors to be analyzed, which may preclude an application when considering the analysis of decision-makers. A new approach to the AHP method was defined by Ren et al. (2018) through decision intervals rather than numerical scales. The use of intervals seeks to improve the uncertainties of the decision-makers' judgment, promoting an analysis and final result with lower associated uncertainties.

The VIKOR method consists of the selection and classification of a set of alternatives, determining the closest solution to the ideal Chatterjee and Chakraborty, 2016). In a study by Ren et al. (2015), the AHP method is used to determine the weights of each evaluated criterion, and the VIKOR method is used for determining the sustainability sequence of the scenarios. Unlike the AHP method, the VIKOR method is not so simple, and is also less popular in studies. However, as the VIKOR method consists of an optimization method, the results of this method, allied with AHP, can improve the quality of the analysis results (Ren et al., 2015).

The MDCA was also associated with the PROMITEE (Mahbub et al., 2019), TOPSIS, and Fuzzy (Onat et al., 2016b) and Threshold value methods (Janjua et al., 2019) (3% of the applied studies). Methods based on Fuzzy analysis are more complex than traditional methods, as they involve a large amount of complex calculations, such as logarithms, and involve more steps for their execution. The PROMITEE method classifies and compares different alternatives through quantitative and qualitative criteria, and its application and interpretation of the results can be easily understood by decision-makers (Mahbub et al., 2019). The TOPSIS method is used in the preference ordering of alternatives according to the distance of the ideal solution—that is, the ideal alternative should have not only the shortest distance of the ideal positive solution, but also the greater distance of the ideal negative solution (Ren et al. 2016c).. In the Threshold value method, the evaluation is based on threshold values of indicators (obtained in the literature), the indicator position on the five-point Likert scale, and the weighting factor (Janjua et al., 2019).

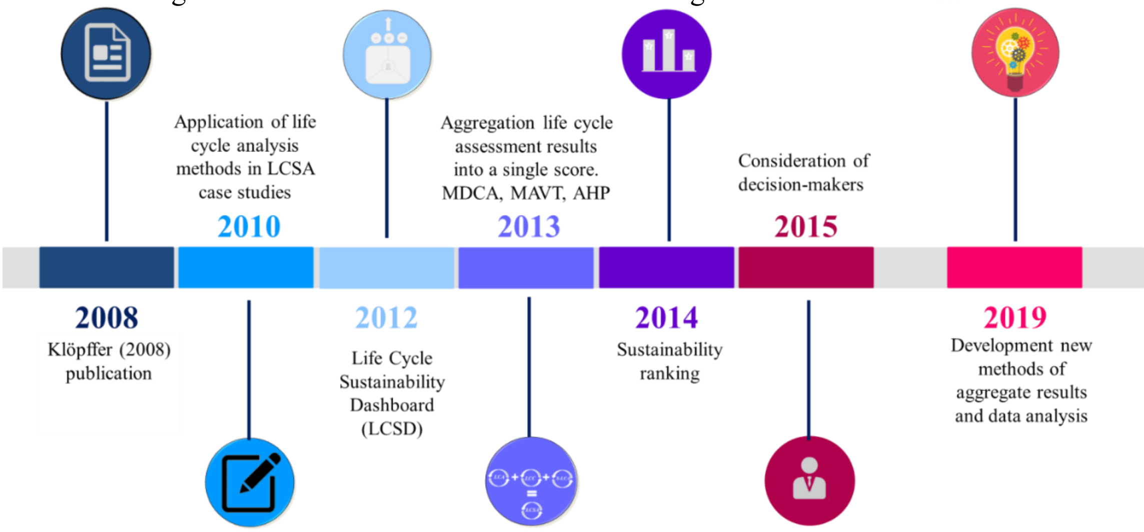
Other aggregation methods were also used as the aforementioned LCSD, applied in 9% of the studies (Traverso et al. 2012a; Traverso et al. 2012b; Schau, Traverso and Finkbeiner, 2012): The multi-criteria classification methods, such as summarization and ranking of the alternatives, were used in 6% of the studies. New methodologies were also developed and applied as the three-dimensional coordinate diagram (Wang et al., 2017), the Interval Multi-Decision Making (MCDM) method (Ren and Toniolo, 2018), Life Cycle Sustainability Performance Matrix (Ren, 2018a), Fuzzy method(Ren, 2018b), and FELICITA model (Kouloumpis and Azapagic, 2018).

The weighting of different indicators is a fundamental process in the MDCA. The weighting factors must be defined, effective, and representative. MDCA methods are used to define these factors normally from a stakeholder group survey. In this sense, 37% of the BP studies considered decision-makers in the sustainability evaluation. The use of decision-makers' analysis aims to minimize the subjectivity of the results, incorporating variability of different groups of stakeholders' visions in the evaluation of sustainability. However, the decision-makers' analysis is time- and resource-intensive, which may hinder their application in practice. In this case, many authors employ different types of weighting, as equals for all criteria evaluated, higher criteria values, and methodologies to define weighting (Chen and Holder, 2018).

The LCSA results of the BP studies that consider the interested parties differ when applying different profiles of decision-makers. This fact highlights that there is not a single answer about which product is more sustainable, or energy source, or even alternative transportation. On the contrary, sustainability depends heavily on the worldview and values of each decision-maker considered in the analysis (Ekener et al. 2018). The LCSA should consider the potential differences of decision-makers in their conclusion, or also include different profiles of decision-makers from around the world in the analysis.

Figure I - 11 illustrates the timeline of the main methodologies and processes employed in LCSA, summing all the detailed information previously. Thus, it is perceived that there is a multitude of methods that have been applied and developed to determine the sustainability of the life cycle by aggregating the results into a single score, with and without the participation of decision-makers in the process. All these methods have different approaches, as well as advantages and limitations. The LCSA methodology still faces many challenges in relation to results integration. It is also verified that there is no ideal method for this aggregation. However, the MCDA method, in combination with the stakeholder profiles, proved to be favorable, considering its greater application. However, the complexity of many of the existing methods is the main obstacle for industry decision-makers to implement LCSA-based methods to assess sustainability (Pesonen and Horn, 2013). Considering that there is still no standardized method for aggregation, and the complexity of many existing methods, it becomes increasingly important to study and develop new methods, applying these in case studies.

Figure I - 11: Timeline of the main methodological events of the LCSA.



Source: own elaboration.

4. Future directions of LCSA studies

LCSA is an important tool in decision-making. Its broad vision of sustainability improves the understanding of the environmental, economic, and social aspects of products and processes. Future research on LCSA should concentrate in three directions: (i) development of analytical methodologies; (ii) selection and measurement of indicators; (iii) use of LCSA in case studies in different sectors and countries.

The development of analytical methodologies for LCSA is an important direction for future research. There is still no universal methodology for LCSA, a fact verified in the numerous methodologies used in BP studies. An interesting way in this direction is to use as a basis the LCA methodology, which is the only standardized and well-disseminated in the scientific community and industry. The LCA programs can serve as a basis for the development of new methods, and also through the elaboration of additional processes to existing programs to analyze economic and social impacts. Thus, the companies that are the developers of these programs can seek methodologies in academia to expand the impact analyses of LCA programs.

Another important factor to be highlighted is that among all LCSA methodologies verified, few understand the use of a single tool for sustainability analysis, such as the Life Cycle Sustainability Dashboard (LCSD). In this sense, future research in terms of methodologies can also advance to the elaboration of a single tool for LCSA. The use of a single tool that results in a unique life cycle sustainability score, or separate results of environmental, economic and social aspects is critical to LCSA. Developing more-simplified methodologies is key to popularizing the use of LCSA by industry decision-makers, governments, and states.

In relation to indicators, future research should: improve the processes of indicators selection, and standardize environmental, economic and social indicators for LCSA; develop more accurate indicator measurement systems; and develop a database relevant to LCSA.

In the systematic analysis, a great variation of selected economic and social indicators was noticed. Thus, future research can act in the development of an oriented and clear process of LCSA indicators selection. Another factor that can be taken into account in the indicators selection is to consider stakeholders. In this sense, future research can also focus on the ecosystem approach towards stakeholder analysis. This type of approach can benefit all actors in the ecosystem for creating and capturing value and therefore using it in the LCSA context. In addition, including stakeholders in the indicator selection process can ensure a more accurate analysis of the study object.

Another factor that can also be explored is a standardization of environmental, economic and social indicators of LCSA. The development of an LCSA methodology with standardized indicators can facilitate the comparison of impacts of different studies, for example. Another important factor is the development of significant economic and social databases similar to environmental databases, such as ecoinvent database. The use of a comprehensive and reliable database improves the LCSA practical use, allowing users the ease in developing lifecycle inventory.

Although the indicators used in BP for economic and social analyses may seem quite independent with easier measurement mechanisms, it is noticed that many indicators are generally quite complex and require more accurate measurement mechanisms. In addition, many of the indicators may require complex production functions for economic analysis and, in many cases, are not entirely independent in social analyses. With this, this understanding of the indicators can be an opportunity for further exploration in the search for more accurate measurement systems in both aspects.

Another direction for future research is in relation to the use of LCSA in case studies in different sectors and countries. Based on the systematic analysis it was verified that there are still many sectorial and local gaps that can be objects of studies applying the LCSA. The sustainability results obtained by a study at a given location may not be the same as in another location. Thus, it is essential to broaden the studies and encompass different sectors in case studies, in order to verify and compare the sustainability of products and services.

In this sense, all sectors highlighted in this research can be evaluated in LCSA case studies in different locations. The electricity and heat production sector can be evaluated in different European countries, yet a global analysis can also be carried out, verifying the most sustainable energy production. The agriculture forestry, and other land use sector can be explored by countries such as the United States, Canada, European and Asian countries. The buildings sector can be evaluated in case studies in South American and African countries. The industry sector can be well explored in case studies involving different production processes both in extraction and also in manufacturing of food, garments, textiles, electronics, non-metallic minerals, and metal products. Another important sector for future research is the environmental remediation (i.e., soil and water), which there are no LCSA studies in this specific sector, only in relation to solid waste. Case studies are fundamental to increasing knowledge and practice, contributing to an acceleration of the development of methodology for LCSA (Sala, Farioli and Zamagni, 2013). In addition, the more case studies are developed, the greater knowledge of the different dimensions of sustainability linked to production.

5. Conclusion

LCSA is an important tool to support decision making, with this analysis it is possible to verify the environmental, economic and social impacts of a given product, service or process. LCSA also assists in the improvement and advancement of cleaner production, sustainability, sustainable development and sustainable production in various sectors of the economy, thus contributing to the implementation of the sustainable development goals in these sectors.

Although there is an increase of publications focusing on LCSA, in literature there are few publications that in practice involve the entire LCSA, involving the three pillars of sustainability. Thus, to determine the current focus of the research in LCSA, firstly this study presents the results of a bibliometric literature by selecting 105 relevant papers for this topic, according to established criteria. Then, the results of the systematic analysis are presented, highlighting the main published studies, the application(s) for each study and localization sector, the indicators and methodologies most used for each dimension of sustainability, and the methodologies employed in the final data analysis. Lastly, the study provides future directions of LCSA studies.

In practice, this research contributes significantly to studies on LCSA. Through a detailed publications analysis it was possible to identify the main Journals, authors and countries that publish on the subject, as well as the main keywords and their interrelations. This type of knowledge guides researchers in the elaboration of new articles on the subject.

Another important factor to be highlighted is the contribution in terms of systematic analysis. In this analysis it was possible to identify the main sectors and countries of LCSA application studies. This analysis guides future research, providing information on which sectors and countries are gaps to explore. In addition, the analysis of the main environmental, economic and social indicators showed that there is great variability in the selection, demonstrating that there is still no standardization of the selection of indicators, especially in economic and social analyses. It is also perceived that, while the LCA is well-developed and normalized, the economic and social analyses still require further studies in order to standardize the methods of analysis selection of indicators. Thus, more opportunities for future research were identified in relation to LCSA indicators.

Finally, the results highlight that in relation to methodologies of sustainability final scores, two forms can be used: through the data of each life cycle analysis in a separate way and with the aggregation of results in a single score. The lack of a standardized methodology for LCSA means that many methodologies are verified both in the analysis of the results in a separate way and also in the aggregation. Another factor to be highlighted is the inclusion of stakeholders in LCSA's sustainability analysis process, through several methodologies. The multi-criteria methods are the most used in both forms. In addition, this analysis demonstrated numerous gaps regarding the need for further studies to develop LCSA methodologies; standardization of a universal methodology for LCSA.

In terms of research limitations, the following aspects need to be considered: (ii) two databases were used for research, which may affect the number of articles, in case of use of other databases; (ii) only articles in peer-reviewed journals, conference papers and book chapters were excluded; (iii) the analysis of the articles was initially done manually, through the reading of titles, abstracts and keywords, this type of procedure may be an unintentional bias in the analysis of the selected works due to the interdisciplinarity of the research team. However, despite these limitations, the results show that the efforts of the scientific community relate in studies of development of methodologies and application in case studies. Thus, it is perceived that sustainability has been a key factor in the search for cleaner and sustainable production, through LCSA it is possible to analyze and improve the sustainability of products, services and processes.

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Supplementary Material

Publications of the bibliographical portfolio:

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Categorization of BP studies by sector

Sector	Application	Reference
Electricity and heat production	Impacts compared of various energy sources	Halog and Manik (2011) Stamford and Azapagic (2012) Stamford and Azapagic (2014) Pesonen and Horn (2013) Ren et al. (2015) Yu and Halog (2015) Atilgan and Azapagic (2016) Huang and Mauerhofer (2016) Akber, Thaheem and Arshad (2017) Ren et al. (2017) Kouloumpis and Azapagic (2018) Ren (2018a) Ren (2018b) Ren et al. (2018) Kabayo et al. (2019) Moslehi and Reddy (2019) Roinioti and Koroneos (2019)
	Sustainability of solar energy	Traverso et al. (2012a) Li, Roskilly and Wang (2018)
	Biogas production and	Jin et al. (2017)
	Hydrogen production	Ren and Toniolo (2018) Valente, Iribarren and Dufour (2019)
	Biorefineries	Keller, Rettenmaier and Reinhardt (2015)
	Biofuels	Collotta et al. (2019)
	Hydro energy	Guo et al. (2019)
	Household energy needs	Gwerder et al. (2019)
Transportation and automobiles	Oxymethylene ether fuel	Mahbub et al. (2019)
	Biomass	Ekener et al. (2018)
	Alternative fuels	Hoque et al. (2019)
	Production of hydrogen from biomass	Stefanova et al. (2014)
	Technological alternatives of vehicles such as electric and hybrid vehicles	Onat, Kucukvar and Tatari (2014a) Onat, Kucukvar and Tatari (2016) Onat et al. (2016a) Onat et al. (2016b) Onat et al. (2016c) Onat et al. (2019)
	Car changer	Schau, Traverso and Finkbeiner (2012)
	Pavement production	Hamdar, Chehab and Srour (2016) Zheng et al.(2019)
	Management of sustainability in automotive companies	Tarne, Traverso and Finkbeiner (2017) Tarne, Lehmann and Finkbeiner (2019) Tarne et al. (2019)
	Battery electric vehicles	Wang et al. (2019)
Industry	Ceramic production	Traverso et al. (2012b) Ferrari et al. (2019) Settembre Blundo et al. (2019)
	Production of high density Polyethylene (PEAD)	Hannouf and Assefa (2017) Hannouf and Assefa (2018)
	Additive manufacturing	Ma et al. (2018)
	Marble	Valdivia et al. (2013)
	Solvent recovery	Zajáros et al. (2018)

	Production of biological-based products	Martin et al. (2018)
	Production of wood-plastic products	Kua (2017)
	Production of magnets for wind turbines	Wulf et al. (2017)
	Productive process of sugarcane biorefinery	Nieder-Heitmann, Haigh and Görgens (2019)
	Macroalgae biorefinery systems	Sadhukhan et al. (2019)
	Production of chemical products	Xu et al. (2017)
Buildings	General construction studies	Ostermeyer, Wallbaum and Reuter (2013) Onat, Kucukvar and Tatari (2014b) Hossaini et al. (2015) Dong and Ng (2016) Gencturk, Hossain and Lahourpour (2016) Wu et al. (2017) Janjua et al. (2019) Liu and Qian (2019)
	Concrete recycling studies	Hu et al. (2013)
	Production of concrete structures	Wang et al. (2017)
	Production of timber for construction	Balasbaneh, Marsono and Khaleghi (2018)
Waste	Municipal waste	Menikpura, Gheewala and Bonnet (2012) Souza et al. (2015) Wang et al. (2018)
	Recycling of bottom ash	Sou, Chu and Chiueh (2016)
	Recycling of cooking oil	Vinyes et al. (2013)
	Anaerobic digestion of source-separated food waste	Iacovidou et al. (2017)
	Disposal scenarios for used polyethylene terephthalate (PET) bottles	Foolmaun and Ramjeawon (2013)
	Waste management Agricultural and Agro Industrial	Aziz, Chevakidagarn and Danteravanich (2016)
	Urban water reuse at various centralization scales	Opher, Friedler and Shapira (2019)
Agriculture, forestry and other land use	Production of soybean	Zortea, Maciel and Passuello (2018)
	Cultivation of olives	De Lucca et al. (2018)
	Dairy production	Chen and Holden (2018)
	Production of animals for consumption	Scherer et al. (2018)
	Use of soil and forests in mangrove management in Thailand	Moriizumi, Matsui and Hondo (2010)
	Alternatives for forest preservation	Pizzirani et al. (2018)
Others	Sustainability of the United Nations' (UN) humanitarian supply chains.	van Kempen et al. (2017)

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3 CAPÍTULO II (artigo de revisão da literatura - publicado): Nano scale zero valent iron production methods applied to contaminated sites remediation: an overview of production and environmental aspects[2]

Abstract: The nano scale zero valent iron (nZVI) is the most used material in the remediation process. The inclusion of sustainability in the remediation process has also been gaining prominence. Sustainable remediation seeks to consider the environmental, economic and social impacts of remediation. Thus, this article aims to: (i) identify and describe nZVI production methods and (ii) evaluate their environmental aspects. Thus, this research was carried out in two stages. The first consisted of systematic bibliographical research to identify and describe nZVI production methods. In the second stage, an environmental analysis of the methods was performed considering the methodology of life cycle inventory assessment. Based on the inventory analysis, a classification of environmental aspects was performed, which included criteria, icons and a color scale. Nine nZVI production methods were identified, which comprised different technologies and processes. All methods had negative environmental aspects, such as high energy consumption, waste, wastewater generation and atmospheric emissions. In the classification of methods with regard to environmental aspects, the milling method had the best score, and the ultrasonic wave method the worst. Overall, this study contributes significantly to the detailed knowledge of nZVI synthesis methods in relation to production processes and their environmental aspects.

Keywords: Synthesis; chemical reduction; energy consumption; sustainable remediation; soil remediation

1 Introduction

The advent of nanotechnology has unleashed enormous potential for the development of new products and applications in various industrial and consumer sectors. In the past 20 years, numerous new technologies have been developed for domestic and industrial application, ranging from drug improvement to new methods for treating contaminated soil and water (Roco and Bainbridge, 2005; Crane and Scott 2012; Deshpande et al. 2020). In this sense, the use of nanomaterials (NMs) in environmental

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[2] *VISENTIN, C., da SILVA TRENTIN, A. W., BRAUN, A. B., THOMÉ, A.. Nano scale zero valent iron production methods applied to contaminated sites remediation: an overview of production and environmental aspects.* ***Journal of Hazardous Materials****, v. 410, p. 124614, 2021. https://doi.org/10.1016/j.jhazmat.2020.124614*

remediation provides economical solutions to some of the most challenging environmental cleaning problems (Zhang 2003; Karn et al. 2009; Peralta-Videa et al. 2011; Adeleye et al. 2016; Zhang et al. 2019).

NMs have the ability to traverse very small pores on the subsurface of soil or remain suspended in groundwater, allowing nanoparticles to react for longer, disperse better, and reach locations farther away than particles (Machado et al. 2015; Gong et al. 2018). Nanoremediation is based on the NMs' properties – i.e. high reactivity and high surface area that enables them to remove a wide spectrum of environmental pollutants such as organohalogenated compounds, hydrocarbons and heavy metals (Ingle et al. 2014; Bakshi and Abhilash 2020; Baragaño et al. 2020; Fajardo et al. 2020). In addition, the use of NMs allows treating contaminated soil and minimizing the addition of more chemicals in the cleaning process (Bardos et al. 2015; Gil-Díaz et al. 2016; Corsi et al. 2018).

In recent decades, NMs have been studied and applied in remediation processes around the world (Saleh et al. 2007; Gomes et al. 2014; Araújo et al. 2015). Among the most common NMs, nano scale zero valent iron (nZVI) stands out as one of the main ones used in remediation, and also as the most studied as it is present in 90% of the studies conducted in this area (Bardos et al. 2015; Cecchin et al. 2016; Visentin et al. 2019, Reginatto et al. 2020).

The production of nZVI can be done through numerous methods that differ in the technologies used, mechanisms and in the processes employed in the production itself (Garnweitner and Niederberger, 2008; Thomé et al. 2015). There are two main technology types: top-down and bottom-up. The former are part of a larger particle size (1 m to 100 µm, for example), such as bulk or powder, that usually undergoes physical processes to obtain nZVI. In the latter, the process occurs in atoms and molecules through chemical reduction reactions (Thomé et al. 2015; Chen et al. 2018; Vaseghi and Nematollahzadeh, 2020). The methods can also be classified according to physical and chemical methods. In the former, nZVI is obtained through physical mechanisms without the occurrence of reactions, while in the latter, reactions are the mechanisms for obtaining nZVI (Bolade et al. 2019; Kolahalam et al. 2019). Currently, many nZVI production methods are being developed mainly in laboratories to reduce production costs and negative environmental impacts, allowing for a broader application of nZVI in practice (Kharisov et al. 2013; Stefaniuk et al. 2016; Bolade et al. 2019).

The nZVI is subject to high Van der Waals forces, and magnetic attraction (Dong and Lo, 2014; Thomé et al. 2015; Chen et al. 2019). Thus, the nZVI has a high reaction capacity and the agglomeration capacity is very high, in its unstabilized form, which results in the reduction of its specific surface, making particles denser than water and reducing the nZVI mobility (Stone et al. 2010; Thomé et al. 2015). So, the use of stabilizers acts in the modification of the nZVI surface characteristics, which can reduce its reactivity, but improves its dispersion and mobility, as well as its remediation properties (Singh et al. 2010; Thomé et al. 2015). The normally used stabilizers are composed of activated carbon generating the carbon-supporting nZVI (Zarei et al. 2014; Bush et al. 2015; Saberinasr et al. 2016; Dong et al. 2017; Cohen et al. 2019); polyacrylic acid, Tween-20, and starch (Dong and Lo, 2014); polyelectrolytes (Jiemvarangkul et al. 2011), Mg-aminoclay (Hwang et al. 2014); Azolla-NaOH (modified aquatic plant filiculoides Azolla) (Arshadi et al. 2017), among others. In addition, the type of stabilizer to be used can be defined based on the characteristics of the compound to be remedied, such as the use of the ramnolipid stabilizer for the immobilization of cadmium and lead in river sediments (Xue et al. 2018); biochar and bentonite for the removal of hexavalent chromium (Shi et al. 2011; Fan et al. 2019).

Although the enormous potential of NMs and nZVI has already been verified in the remediation of contaminated sites and the use is already consolidated, the environmental behavior of NMs is not sufficiently known (Fulekar et al. 2014; Khin et al. 2012; Patil et al. 2016; Visentin et al. 2019; Bartolozzi et al. 2020). Knowledge of the environmental impacts associated with NMs is extremely important to assess their sustainability in remediation. Over the last few years, the inclusion of sustainability in remediation has made decision makers' concerns stem not only from the remediation results, but also from the environmental, economic and social impacts that remediation can cause (Elis and Hadley, 2009; Sierra et al. 2016; Braun et al. 2019).

It was found that only three studies have performed an environmental impacts analysis of nZVI synthesis methods (Martins et al. 2017; Joshi et al. 2018; Visentin et al. 2019), and a study evaluated the life cycle sustainability of nZVI production methods (Visentin et al. 2021). Martins et al. (2017) evaluated the traditional methods of chemical reduction with sodium borohydride, and green synthesis through production using plant extracts. Johsi et al. (2018) analyzed the impacts of the green synthesis method with microbial reduction of natural Fe (III) while Visentin et al. (2019) and Visentin et al. (2021) evaluated the methods of milling, reduction with sodium borohydride and reduction with hydrogen gas. However, these studies evaluated only a portion of nZVI production methods.

This paper contributes to the current research on nZVI and sustainable remediation by: (i) describing in detail nZVI production methods; (ii) presenting the production processes of each method, inputs and outputs such as energy and water consumption, and generation of waste, effluents and emissions; and (iii) evaluating the environmental aspects of nZVI production methods and determining an environmental ranking of the methods. In practice, this article seeks to address the gap in the literature around the knowledge of the environmental aspects of nZVI synthesis methods.

Thus, the aim of this work is to identify and describe nZVI production methods and to analyze the environmental aspects of the production methods, thereby determining an environmental ranking.

2 Methodology

This research was carried out in two stages: the first comprised identifying and describing nZVI production methods, and in the second, a detailed analysis of the production methods, namely the production process, necessary inputs, waste, wastewater and generated emissions, was performed. Additionally, in the second stage, a semi-qualitative classification of the methods' environmental aspects was made with different icons and a color scale.

The methods were identified through a systematic bibliographic review of publications on nZVI production methods. This research was carried out on the pages of the worldwide computer network through research in the databases of scientific journals, such as Scopus, Web of Science, Science Direct, and others. The search was performed with keywords related to nZVI production methods, including: "nZVI production methods/nano scale zero valent iron production methods", "nZVI synthesis methods/nano scale zero valent iron synthesis methods", "nZVI life cycle analysis/nano scale zero valent iron life cycle analysis", along with others relevant to the scope of this stage goal.

According to Levy and Ellis (2006), the goal of systematic review is to create a theoretical-scientific basis on a given topic or subject through the process of mapping, collecting, knowing, understanding, analyzing and synthesizing a set of published scientific papers. Furthermore, according to Brereton et al. (2007), a systematic review allows the researcher to perform a rigorous and reliable evaluation of the research conducted within a specific theme.

The second stage was performed with production methods analysis. A survey of all inputs and outputs in each method was realized in a detailed analysis of the production process, where the theoretical principles of Life Cycle Inventory Assessment (LCIA) were considered in order to guide a more representative and accurate analysis.

Life Cycle Assessment (LCA) is an environmental impact analysis tool for the life cycle of a given product/service/process. However, the LCIA is a part of the LCA that analyzes the inventory of a product, in this case that of each nZVI production method. In a complete LCA analysis, its first step is to define the system limit to be evaluated, which in this case is nZVI production through different methods. At this stage, it is still essential to define the functional unit, which in this case is 1.00 kg of nZVI produced by each production method. All inventory inputs and outputs are based on the functional unit. Thus, the survey of information about the inputs and outputs of the methods was based on this unit. In the second stage of a LCA, the inventory analysis is made and all the inputs and outputs of the methods production processes are quantified – i.e. the amount of reagents, water and energy, the amount of solid waste generated, wastewater and emissions. The inventory data of the production methods is displayed in the supplementary material.

Based on the information from the life cycle inventory analysis of each production method, a comparative analysis was made between the methods in relation to different environmental aspects. Thus, a semi-quantitative environmental classification was proposed for production methods in the following aspects: inputs (reagents and materials), water consumption, energy consumption, waste generation, wastewater generation and atmospheric emissions. The environmental aspects were selected based on the LCA methodology. To perform an environmental impacts analysis of the methods through an LCA it is necessary to obtain information about all inputs and outputs of the production processes, and this information was categorized in the environmental aspects of this study.

For each environmental aspect, icons and a classification color scale were defined according to specific criteria. Environmental aspects are classified in the color scale according to the characteristics of the input compounds and emissions as well as the amounts of water and energy consumption, and the amount of waste and wastewater generated by each method. The color scale consists of three colors: green, yellow, and red. In general, green indicates positive or low environmental aspects (compounds with less danger to human health, lower amount of water and energy consumption, and generation of waste and wastewater), yellow, moderate environmental aspects (moderate health effects and average amounts of consumption and generation of waste and effluents), and red, negative environmental aspects (compounds that affect human health, high water and energy consumption, higher amount of waste and wastewater). Table II - 1 summarizes the environmental aspects considered, the icons of each aspect, and the classification criteria for the color scale.

The classification criteria of each environmental aspect were defined based on inventory analysis results. With regard to inputs, the characteristics of the reagents and materials were considered to define the classification, based on the Globally Harmonized System of Classification and Labelling of Chemicals (GHS) (Winder et al. 2005; Yazid et al. 2020). With regard to water consumption, energy consumption, the amount of water and energy consumed, and wastewater and waste generated, each method was used in the definition of classifications. With atmospheric emissions, the characteristics of the emissions defined the classification.

Table II - 1: Classification criteria of the environmental aspects of nZVI production methods.

Method	**Description**	**Diameter (nm)**	**Surface area (m^2/g)**	**References**
Milling	Grinding iron particles in a high-speed rotating chamber	10 - 50	39.0	Li, Yan and Zhang (2009)
Liquid chemical reduction	Reduction of iron sais using liquid reducing agent	1 - 100	30	Wang e Zhang (1997); Sun et al. (2006)
Gaseous chemical reduction	Reduction of iron sais using gas reducing agent	40 - 70	29	Uegami et al. (2009)
Thermal reduction	Reduction of Fe^{+2} at high temperatures with the use of thermal energy in the presence of gaseous reducing agents	20 - 150	130.0	Hoch et al. (2008); Dai et al. (2016)
Chemical vapor deposition	Vaporization of the target material by heat sources stops after being condensed quickly	25	40 – 60	Dumitrache et al. (2004)

Method	Description	Diameter (nm)	Surface area (m^2/g)	References
Micro-emulsion	Use of an inorganic phase in micro water emulsions in oil	40 - 60	20 – 60	Li, Vipulanandan and Mohanty (2003), Zhang et al. (2007)
Ultrasonic waves	Use of ultrasound waves and reducing agent	10	34.0 – 42.0	Jamei, Khosravi e Anvaripour (2013)
Electrochemical	Reduction of iron salt by electric current	1 – 20	25.4	Chen et al., (2004)
Green synthesis	Biosynthesis using plant extracts or microorganisms	20 - 120	5.8	Martins et al. (2017) Bolade, Williams and Benson (2019)

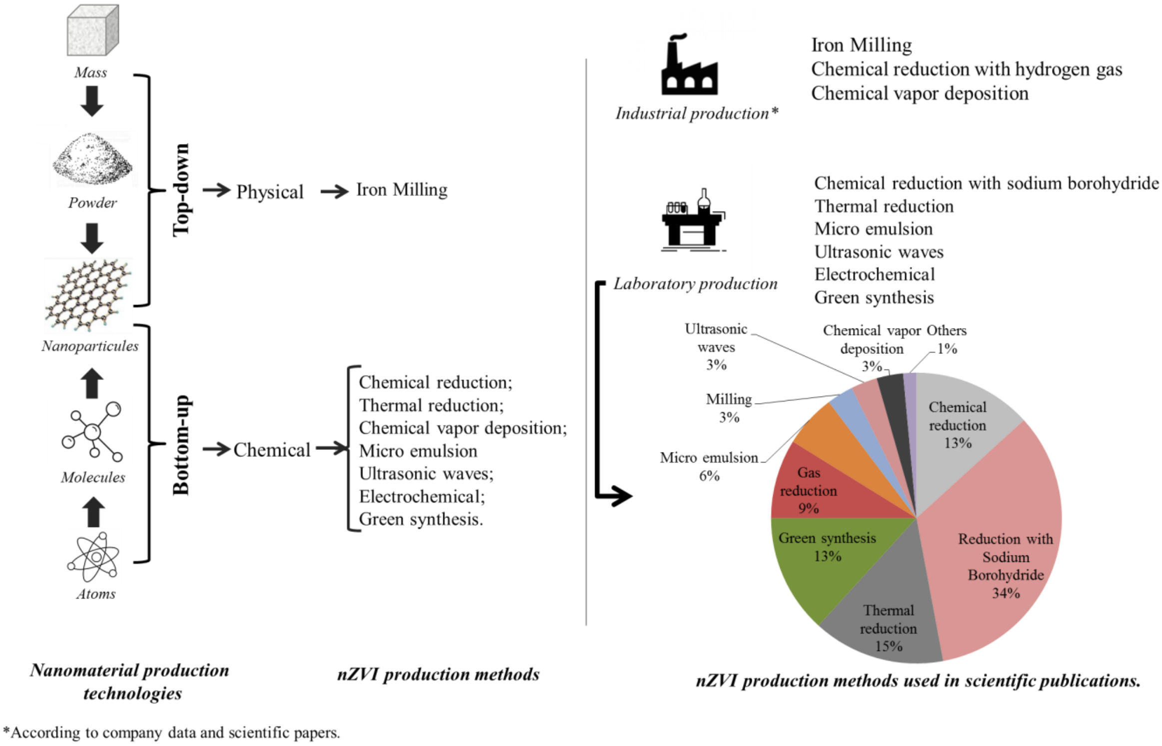
The information was organized in a spreadsheet for grouping and performing a comparative analysis between production methods. This type of analysis was based solely and exclusively, for classification purposes, on the level of satisfaction of both environmental aspects and methods. For each classification in the color scale, values were assigned in order to provide a final classification of methods with regard to the environmental aspects. The defined score scale ranged from 0.00 to 3.00 and was defined based on the methodologies of Finkbeiner et al. (2010), Traverso et al. (2012) and Zortea et al. (2019). The green icons represented a score of 3.00, the yellow icons, of 2.00, and the red icons, of 0.00. At the end, a simple sum of these scores defined the environmental classification of the methods.

A similar approach with color and numerical scale was used by Ridsdale and Noble (2016) who point out that although qualitative analyses are simple in its design, it provides a quick evaluation. It allows for the evaluation of strengths, the main aspects that can generate negative environmental impacts on the methods, and areas where improvements are still needed.

3 The nZVI production methods

Nine nZVI production methods were identified: milling, liquid chemical reduction with sodium borohydride, gaseous chemical reduction with hydrogen gas, thermal reduction, chemical vapor deposition, micro-emulsion, ultrasonic waves, electrochemical and green synthesis (Figure II - 1). These methods include physical and chemical processes and top-down and bottom-up technologies.

Figure II - 1: The nZVI production methods, production technologies and scale used in scientific publications.



Of the methods identified, only the milling method comprises a physical process from the top-down. The other methods are bottom-up technologies and chemical methods. Among them, we gained knowledge, through data published by the companies producing nZVI and scientific publications, about the use of three methods in the industrial production of nZVI: milling, chemical reduction with hydrogen gas and chemical vapor deposition (Crane and Scott, 2012).

Most methods are developed and used only in laboratory production. In scientific publications, the most used methods in nZVI production are: chemical reduction with sodium borohydride (34%), thermal reduction (15%), green synthesis (13%), gas reduction (9%), micro-emulsion (6%), and other methods such as milling, chemical deposition, ultrasonic waves, electrochemical, etc. correspond to 23% of the applications in the studies. Table II - 2 presents a detailed summary with the main information about nZVI production methods, such as production process characteristics, diameter of nanoparticles produced and specific surface area.

Table II - 2: The nZVI production methods, their characteristics and properties.

Environmental aspects	**Icons**	**Classification criteria**
Inputs (reagents and materials)		Green: materials harmful to the environment and human health.
		Yellow: materials that present some risk to the environment and human health, with characteristics such as corrosive and irritant.
		Red: materials that are at high risk to the environment and human health, with characteristics such as acute toxic, health hazard, flammable.
Water consumption		Green: water consumption during the production process from 0 to 0.03 m³.
		Yellow: water consumption during the production process of 0.031 to 0.07 m³.
		Red: water consumption during the production process above 0.71 m³.
Energy consumption		Green: energy consumption during the production process from 0 to 30 kWh.
		Yellow: energy consumption during the production process from 31 to 60 kWh.
		Red: energy consumption during the production process above 61 kWh.
Solid waste generation		Green: no waste generated.
		Yellow: waste generation during the production process of 0 to 1.0 kg. Waste generated has some harmful effect on the environment and human health, requiring proper final disposal.
		Red: waste generation during the production process above 1.1 kg. Waste generated is at high risk to the environment and human health, requiring proper final destination.

Environmental aspects	Icons	Classification criteria
Wastewater generation		Green: wastewater generation during the production process from 0 to 0.03 m³.
		Yellow: wastewater generation during the production process of 0.031 to 0.06 m³.
		Red: wastewater generation during the production process above 0.06 m³.
Atmospheric emission		Green: atmospheric emissions of harmful compounds such as water vapor.
		Yellow: atmospheric emissions of compounds that present some risk to the environment and human health.
		Red: atmospheric emissions that present a high risk to the environment and human health.

3.1 Milling

The milling method is characterized as a top-down physical production technique. The production of nZVI is carried out with equipment that promotes the grinding of particles, such as a high-speed rotating chamber, planetary ball mill systems, and others. The milling system consists basically of two subsystems: (1) the milling system, comprising an engine, a grinding chamber, an agitator and steel balls, and (2) a particle circulation and cooling system, containing a pump and a retaining tank to control the temperature of the iron suspension in the tank and inside the mill. The iron microparticles are inserted into the grinding chamber together with steel balls (250 μm in diameter), which consist of the nZVI forming medium. The mass ratio of steel spheres and particles ranges from 20:1 to 40:1 depending on the methodology and equipment used (Ioannou et al. 2012; Jung et al. 2015)

During milling, the motor drives the agitator at a determined rotating speed in order to stir the milling medium (balls and iron particles with size of 1-50 μm). The iron particles are crushed by the steel spheres, and the impact energy fractures the material into smaller pieces. The rotating chamber contains a cylinder that acts as a filter to retain the steel balls, but allows the passage of the processed iron material to the retaining tank, in which the iron particles return to the milling system by the circulation pump until they reach the established diameter. The obtained nZVI is collected at the exit of the milling process (Li et al. 2009). During the process, mechanical wear of iron particles occurs until they reach their nanometric size.

The milling method can be operated under both dry and humid conditions. Dry milling is performed using only milling balls and iron particles, while in wet milling, reagents are added to this process. In the former process, the typical parameters that affect the particles' physicochemical properties are the milling equipment type, energy, time, ball and powder ratio, particle stiffness and feed size. In the latter process, suspension properties, such as viscosity, solid concentrate and pH, should be considered in addition to the powder properties (Jung et al. 2015).

3.2 Liquid chemical reduction with sodium borohydride

Chemical reduction is the most widely used nZVI production method, in which, through chemical reactions, iron sais is reduced with the application of reducing agents. In liquid reduction, sodium borohydride ($NaBH_4$) is the most used reducing agent, mainly in laboratory scale studies, due to its simplicity.

The synthesis of nZVI occurs by mixing equal volumes of iron chloride aqueous solutions ($FeCl_3$) and sodium borohydride aqueous solution ($NaBH_4$). The latter is added to the former at a controlled drop-by-drop rate under continuous agitation at room temperature for about 20 minutes (Kanel et al. 2005; Martins et al. 2017; Barreto-Rodrigues et al. 2017). The nZVI particles appear immediately after the addition of the first drops of the reducing agent solution (Barreto-Rodrigues et al. 2017). In order to be used in environmental remediation, the obtained nZVI must be filtered, washed and dried (Sun et al. 2006; Barreto-Rodrigues et al. 2017). The separation is usually performed through vacuum filtration, washing is done with deionized water, ethanol or acetone, and drying under inert atmosphere. Washing with ethanol and acetone is used to avoid immediate oxidation of the nZVI during purification, leading to a fine black powder product (Kanel et al. 2005). Ferric iron (Fe^{+3}) is reduced to zero valence, according to the reaction expressed in Equation 1 (Sun et al. 2006).

$$4Fe^{3+}_{(aq)} + 3BH_4^- + 9H_2O_{(aq)} \rightarrow 12Fe^0_{(s)} + 3H_3BO_{3\,(aq)} + 12\,H^+_{(aq)} + 9H_{2(g)} \quad (1)$$

3.3 Chemical gas reduction with hydrogen gas

The main method of gas reduction is with the use of hydrogen gas as a reducing agent. Here, the synthesis of nZVI is made by reducing goethite and hematite particles at high temperatures with hydrogen gas (O'Carroll et al. 2013), according to the reaction expressed in Equation 2 (Kuila et al. 2016).

$$Fe_3O_{4(s)} + 4H_{2(g)} \rightarrow 3Fe^0_{(s)} + 4H_2O_{(g)} \quad (2)$$

The first stage of nZVI synthesis is the production of goethite (α-FeO/OH) and hematite (α-Fe_2O_3) particles. The former can be obtained through common methods by passing an oxygen-containing gas through a suspension containing a ferrous precipitate (iron hydroxides or carbonates) that is obtained through reaction with an aqueous solution containing ferrous salts and compounds such as alkaline hydroxides, alkaline carbonates, etc. (Uegami et al. 2009). Purification of the aqueous solution is essential to limit the amount of impurities in goethite particles. Hematite particles, in turn, are obtained through heat dehydration of goethite particles at a temperature of 250 to 350 °C (Uegami et al. 2009).

After this process, goethite and hematite particles are reduced by heat at a temperature of 350 to 600 °C in a hydrogen gas atmosphere (Uegami et al. 2009). The obtained nZVI particles are cooled, removed and transferred to water, avoiding the formation of an anoxidation film on the nZVI particles surface in the gaseous phase (Uegami et al. 2009). After oxidation, the particles are dried in greenhouses with a temperature not exceeding 100 °C. After drying, nZVI is obtained.

The process of goethite and hematite particles reduction with heat results in iron particles composed of α-Fe^0 phase as a whole. According to Uegami et al. (2009), by transferring iron particles to water, the latter is decomposed into oxygen and hydrogen by the catalytic activity of α-Fe^0. The resulting nZVI particles have two phases consisting of α-Fe^0 and Fe_3O_4 generated by oxidation with water.

In a laboratory scale, the method is performed in a thermogravimetric analysis device. The magnetite ores are arranged in a crucible and placed in the thermogravimetric analysis device, with the temperature in an argon atmosphere increasing gradually. When the reaction temperature is reached, the hydrogen gas is inserted into the appliance. Once the reduction reaches completion, the hydrogen flow is stopped and the argon flow resumes. The reduced powder is cooled in the argon atmosphere and removed from the system at about 300 and 400 °C (Kuila et al. 2016).

3.4 Thermal reduction

Thermal reduction, better known as carbothermal reduction, is one of the methods investigated for the production of cheap and functional nZVI (Crane and Scott 2012). In this method, the gaseous Fe^{+2} oxide particles or salts are reduced in high temperatures with the use of thermal energy in the presence of gaseous reducing agents, such as H_2, CO_2 or CO produced during the thermal decomposition of materials-based carbon (black carbon, biochar, nano carbon particles) (Stefaniuk et al. 2016). According to Equations 3 and 4 (Hoch et al. 2008), Fe^0 is formed as a result of a high temperature endothermic reaction (>500°C).

$$Fe(C_2H_3O_2)_{2\,(aq)} + C_{(s)} \rightarrow Fe^0_{(s)} + 2CH_2CO_{(g)} + CO_{(g)} + H_2O_{(g)} \qquad (3)$$

$$Fe_3O_{4(aq)} + 2C_{(g)} \rightarrow 3Fe^0_{(s)} + 2CO_{2(g)} \qquad (4)$$

Initially, the solution of the carbon source with deionized water is mixed by agitation, after which a solid forms and is separated from the supernatant solution through vacuum filtration (Hoch et al. 2008). The solid is removed from the filter while still in a mild state of solidification, and placed in a vacuum oven, without heating, for a few hours to dry – about 12 hours, according to Hoch et al. 2008. After drying, the resulting samples are charred in a tube oven heated in nitrogen flow for approximately three hours (Dai et al. 2016). The heating temperature can range from 500 to 1,000 °C. After this process, the samples are cooled to room temperature naturally, thus obtaining nZVI supported by carbon (C-Fe^0) (Hoch et al. 2008; Dai et al. 2016; Orlandi et al. 2017).

In this method, nZVI is encapsulated in carbon, resulting in a lower aggregation of particles (Hoch et al. 2008), and a relatively higher degradation capacity compared to its version without encapsulation, as evaluated by Dai et al. (2016) and Hoch et al. (2008) in the reduction of hexavalent chromium.

According to Orlandi et al. (2017), carbothermal reduction can be performed with any carbon source, the most common being carbon black, although it has also been done with the use of graphite, carbon nanotubes or even sugar. However, there are still gaps on the efficiency of synthesis using different carbon sources (Orlandi et al. 2017).

3.5 Chemical vapor deposition

The steam chemical vapor deposition method consists of a vaporization process in which the target materials are initially vaporized with heat sources after being quickly condensed (Tavakoli et al. 2007). Besides being applied in the production of nanomaterials, mainly carbon nanotubes, this method is commonly used in the manufacture of coating films in various products (Park and Sudarshan 2001).

The chemical vapor deposition method can be subdivided into physical and chemical methods, the former comprising processes in which nano particles have the same composition as the target material (Park and Sudarshan 2001; Tavakoli et al. 2007), while the latter occurs through reactions that modify the composition of the target material for nanomaterials formation (Park and Sudarshan 2001; Tavakoli et al. 2007). The chemical deposition method is the most used for the manufacture of nZVI.

In the chemical vapor deposition method, reactions occur between the steam and other system components during the vaporization and condensation steps. It is performed by means of a vacuum-maintained high purity reactive gas chamber in which reactions occur, and an operational precursor delivery system at ambient pressure. The precursor consists of the target material of the process, in this case nZVI. The gas chamber and collection system are connected by means of a valve that controls and monitors the process (Tavakoli et al. 2007).

The method operation comprises the insertion of reagents – a precursor material, the reducing agent and the gas – in the reaction chamber. The reagents used are iron pentacarbonyl, argon gas, ethylene, acetylene and ethyl. The chamber is heated, and the synthesis reaction forming the nZVI occurs for a short period. In the chamber outlet tube, the gas current is rapidly expanded in two phases – gas and nanoparticles – to avoid the growth and agglomeration of the nanoparticles. After the nanoparticles condense into a rotating substrate of liquid nitrogen, they are transferred to the delivery system, where they can be scraped and collected. The vaporization process causes structural changes in particles, such as purification and crystallization, as well as transformation to a desirable size, composition and morphology (Tavakoli et al. 2007).

3.6 Micro-emulsion

Many authors have considered micro-emulsion as a method of modifying nZVI to improve its characteristics (Stefaniuk et al. 2016). However, other authors used this method in the production of nZVI particles (Li et al. 2003; Capek 2004; Zhang et al. 2007; Malik et al. 2012; Beygi and Babakhani 2017).

The micro-emulsion method consists of an inorganic phase in micro water emulsions used in oil for the preparation of uniform metallic particles (Tavakoli et al. 2007). It is a single phase composed of at least three components: two of them are non-miscible, such as water and oil, and the third, a surfactant at the water/oil interface (Tavakoli et al. 2007). Micro emulsions can occur in two ways: (1) by means of oil micelles dispersed in the aqueous phase (oil/water micro-emulsion – O/W), or (2) in water micelles dispersed in oil (micro-emulsion water/oil – W/O, or reverse micro-emulsion).

The nZVI synthesis occurs in reverse micelles, called micro reactors, through numerous micro drops of water distributed in an organic phase by means of a surfactant (Capek 2004; Beygi and Babakhani 2017). In this method, the size and morphology of synthesized particles are controlled through the method parameters, such as the size of water droplet molecules (Capek 2004; Tavakoli et al. 2007; Beygi and Babakhani 2017).

For the method application, it is necessary to initially determine the composition of micro emulsions and surfactants based on the product to be obtained (Zhang et al. 2007). After this process occurs, the mixture of these micro emulsions, one of which contains the metallic precursor (i.e. ferric chloride) and the other, the precipitating agent (i.e. sodium borohydride), is carried out, during which both reagents come into contact with each other due to droplet and coalescence collisions, and react to form precipitates of nanometric size (Sanchez-Dominguez et al. 2012). The exchange between the reagents is very fast and can occur, in a matter of seconds, only during the mixing process (Capek 2004). Synthesis reactions occur within droplets, which control the final particle size (Capek 2004).

During the reduction reaction, a gas and a solid with black coloration are formed in the solution (Li et al. 2003). The formed gas is evolved in collection systems. After this process, agitation occurs again, and then the material is centrifuged to separate the nZVI (Li et al. 2003). These particles are washed with ethanol or acetone and then removed. The removal of nZVI can be performed through numerous methods, such as the *in situ* deposition method (Ohde et al. 2001), the RESS method (Rapid Expansion of

Supercritical Solution) (Ji et al. 1999), and also through magnets (Li et al. 2003; Capek 2004). The entire production procedure must be carried out in a nitrogen atmosphere.

The average size of nanoparticles synthesized by the micro emulsion method depends on the size of the micro-emulsion drop used in the process, the concentration of reagents (especially the surfactant), and also on the flexibility of the surfactant film with the nanoparticles (Capek 2004).

3.7 Ultrasonic wave method

The ultrasonic wave method consists of the use of waves to improve nZVI production through physical and chemical methods of synthesis (Stefaniuk et al. 2016). Ultrasonic waves help reduce particle size, and increase surface area and uniformity (Jamei et al. 2013; Stefaniuk et al. 2016). This method is mainly applied on a laboratory scale in conjunction with other methods, such as reduction with sodium borohydride. Thus, nZVI synthesis occurs by basically following the same process as reduction synthesis with sodium borohydride.

The synthesis of nZVI initially occurs with the preparation of Fe^{+3}, $NaBH^4$ and ammonium hydroxide solutions with deionized water. These solutions are transferred to a balloon reactor with three open necks. Ultrasonic waves are applied through a titanium probe submerged in the solution, with a constant frequency (e.g. 20 kHz) and power that can range from 0 to 1,000 Watts (Jamei et al. 2013). In the other bottle, necks are injected with nitrogen gas and argon to remove oxygen and prevent oxidation in the process. The reaction balloon should be submerged in water to maintain the solution temperature, since the latter increases during the reaction in the presence of ultrasonic waves (Jamei et al. 2013). The formed nZVI is filtered through a membrane filter and then washed with pure ethanol, after which the nZVI is placed in a centrifuge to remove moisture. The resulting solids are dried in a vacuum oven for at least 24 hours and then stored in a refrigerator to avoid oxidation.

In this method, ammonium hydroxide is added to the solution to avoid nZVI oxidation caused by the release of hydrogen during the production reaction, and the amount of nZVI produced is increased (Jamei et al. 2013). The reaction of the ultrasonic wave method with the chemical reduction and sodium borohydride occurs according to the reaction expressed in Equation 5 (Jamei et al. 2013).

$$4Fe^{2+}_{(aq)} + BH^{-}_{4(aq)} + 7NH_4OH_{(aq)} \rightarrow 4Fe^{0}_{(s)} \downarrow + H_3BO_{3(aq)} + 7NH^{+}_{4(aq)} + H_2O_{(g)} \quad (5)$$

3.8 Electrochemical method

The electrochemical method is based on the application of electrolysis in nZVI production through solutions containing iron sais (e.g. Fe^{+2} and Fe^{+3}), electrodes (cathodes and anodes) and electric currents (Stefaniuk et al. 2016). The method proposed by Chen et al. (2004) combines electrochemical and ultrasonic techniques.

The nZVI is formed by reducing ferric chloride according to the reactions expressed in Equations 6 and 7 (Chen et al. 2004). The nZVI atoms produced are gradually deposited in the cathode. However, they present a strong tendency towards agglomeration (Chen et al. 2004; Stefaniuk et al. 2016). Thus, cationic surfactants, acting as stabilizing agents, are used, as well as ultrasonic waves, which constitute a necessary energy source for the rapid removal of nZVI from the cathode (Chen et al. 2004).

$$Cathode: Fe^{+3} + 3e^{-} + stabilizer \rightarrow nFeZ \quad (6)$$

$$Anode: Cl^{-} \rightarrow \frac{1}{2}Cl_2 + e^{-} \quad (7)$$

The production of nZVI initially occurs with the preparation of the ferric chloride solution. In an electroplating reactor, the method is assembled, and the electrodes must be lined with inert material to avoid the occurrence of reactions between the nZVI produced and the electrode. The electroplating reactor is then arranged inside an ultrasonic vibrator with water inside, which aids in the removal in nZVI of the cathode before grouping and is used simultaneously during the reaction to provide physical energy for the removal (Chen et al. 2004). The iron chlorine solution (III) is transferred to the reactor, and is added together with the stabilizers (e.g. Polyvinylpyrrolidone (PVP) and Cetylpyridinchloride (CPC)) to avoid grouping the nanoparticles. The nZVI produced must be collected under oxygen-free water, thus the use of argon.

3.9 Green synthesis

The use of green synthesis methods has been growing in recent years. These methods have emerged as an alternative to the traditional chemical and physical methods of nZVI production, mainly due to high production costs (Yadav et al. 2017). Thus, in addition to lower costs, green synthesis is also an eco-friendly method when compared to traditional methods that result in high energy and resource consumption, in addition to generating waste, wastewater and emissions that require treatment and disposal-appropriate ends (Bolade et al. 2019).

Green synthesis can occur through plant extracts and microorganisms, such as fungi and bacteria, in a bottom-up approach. Microbial enzymes or plant phytochemicals, with antioxidant or reducing properties, are generally responsible for the reduction and oxidation of metallic compounds (Yadav et al. 2017). The compounds present in these extracts react with iron (III) in the solution to form nZVI (Machado et al. 2013).

The green synthesis with plant extracts is mainly made of those with high polyphenol sums and high antioxidant capacity, such as coffee plants, green tea, black tea, lemon, balm, sorgo, bran, grape, etc. (Machado et al. 2013; Stefaniuk et al. 2016). According to Machado et al. (2013), fruit tree leaves are considered promising agents for nZVI production.

The green synthesis method using microorganisms is not yet widespread in the scientific community. In addition, the use of microorganisms in nZVI synthesis requires the mandatory restriction of aseptic conditions, which demands trained personnel, and so increases production costs (Stefaniuk et al. 2016). Another factor is the reaction time, which in the synthesis with microorganisms is greater than that with plant extracts. Thus, the use of plants for green synthesis ends up being preferable over microorganisms (Stefaniuk et al. 2016).

The green synthesis method with plant extracts is quite simple, and comprises the preparation stage of the polyphenolic solution, which occurs by heating plant extracts in water to a temperature close to boiling point. These extracts may be crushed or in their natural form (Machado et al. 2013; Stefaniuk et al. 2016; Martins et al. 2017). Afterwards, the separation of the plant residue extract occurs and is mixed with a Fe^{+2} solution. Iron ions in the presence of polyphenols are reduced to Fe0. The residues generated in this method are sheets and filters of paper, and these must be disposed of properly in landfills or incinerators since they may contain iron compounds like the wastewater generated in this method (Martins et al. 2017).

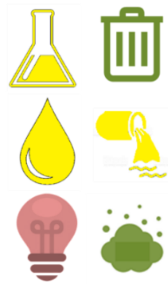
Green synthesis methods can be easily applied on an industrial scale since they do not require the use of high temperatures, pressure or additional energy inputs, on top of low cost (Stefaniuk et al. 2016). However, many authors affirm the need for further studies to understand the production and application processes, the physicochemical properties, reactivity and agglomeration of the nanoparticles produced (Machado et al. 2013; Stefaniuk et al. 2016). In addition, during the synthesis process, incomplete reduction of iron to nZVI may occur, resulting in the formation of other forms of iron and iron oxides (Huang et al. 2014; Stefaniuk et al. 2016).

4 Environmental aspects of nZVI production methods

Table II - 3 presents a summary of synthesis methods in relation to their production, environmental classification, benefits and limitations. In this table, the production processes of the methods and their steps are presented in detail, as well as the inputs and outputs. The classification of environmental aspects is also shown through each icon (inputs, water, energy, waste, wastewater and emissions) and the color scale described in the methodology.

Table II - 3: The nZVI production methods: production processes, inputs and outputs, environmental classification.

Methods	Production process stages	Inputs	Outputs	Environmental classification	References
Milling	Milling	Iron particles Energy	Atmospheric emissions (particulate matter)		Li et al. (2009); Visentin et al. (2019)
Liquid chemical reduction with sodium borohydride	Mixing of reagents and washing	Iron chloride (III) ($FeCl_3$) Sodium borohydride ($NaBH_4$) Deionized water Ethanol Energy	Wastewater		Wang e Zhang (1997); Sun et al. (2006); Martins et al. (2017); Visentin et al. (2019)
	Filtration and drying	Energy Paper filters	Wastewater (with boron produced)		

Methods	**Production process stages**	**Inputs**	**Outputs**	**Environmental classification**	**References**
Gaseous chemical reduction with hydrogen gas	Production of goetite and hematia particles	Sodium carbonate ($NaCO_3$) Iron sulfate (II) ($FeSO_4$) Nitrogen (N_2) (gas) Iron carbonate ($FeCO_3$) Aluminium hydroxide $Al(OH)_3$ Energy	Solid waste Wastewater		Uegami et al. (2009); Visentin et al. (2019)
	nZVI synthesis (reduction, oxidation and drying)	Goetita and hematonite Gaseous hydrogen (H_2) Nitrogen (N_2) Deionized water Energy	Wastewater		
Thermal reduction	Reagentes mixing	Iron nitrate (III) $Fe(NO_3)$ Carbon black Deionized water Energy			Hoch et al. (2008); Dai et al. (2016)
	Filtration and drying	Nylon membrane Energy	Wastewater Solid waste (with carbon presence)		
	Carbonization	Iron(III) Acetate $Fe(C_2H_3O_2)_3$ Argon Energy	Atmospheric emissions (containing argon, ketene (CH_2CO), carbon monoxide (CO), carbon dioxide (CO_2), water vapor)		

Methods	**Production process stages**	**Inputs**	**Outputs**	**Environmental classification**	**References**
Chemical vapor deposition	nZVI syntesis	Iron pentacarbonyl ($Fe(CO)_5$) Ethyl (C_2H_5) Ethylene (C_2H_4) Acetylene (C_2H_2) Argon Energy	Atmospheric emissions (particulate matter, argon, carbonates)		Dumitrache et al. (2004)
Micro-emulsion	nZVI synthesis (preparation of micro emulsions, mixing and separation)	Iron Sulfate (II) ($FeSO_4$) Borohydride potassium (KBH_4) Surfactant n-butanol Iisooctane Deionized water Argon Energy	Wastewater		Li et al. (2003), Zhang et al. (2007)
	Washing and drying	Deionized water Anhydrous ethanol Acetone Argon Energy	Solid waste Wastewater		
Ultrasonic waves	nZVI synthesis (preparation of reagents and agitation with ultrasonic waves)	Iron Sulfate (II) ($FeSO_4$) Sodium borohydride ($NaBH_4$) Ethanol Nitrogen Deionized water Energy	Wastewater (with sodium sulfate and boric acid) Atmospheric emission (hydrogen gas H_2)		Jamei, Khosravi e Anvaripour (2013)
	Filtration, washing and centrifugation	Ethanol Nylon filter membrane Energy	Wastewater Solid waste		

Methods	Production process stages	Inputs	Outputs	Environmental classification	References
Electrochemical	nZVI synthesis (reagent preparation, synthesis and collection)	Iron chloride (III) ($FeCl_3$) Deionized water Stabilizers (e.g., polyvinylpyrrolidone (PVP), cetylpyridin chloride (CPC)) Argon Energy	Wastewater Atmospheric emissions (containing chlorine gas)		Chen et al., (2004)
Green synthesis (with plant extracts)	nZVI synthesis (sheet grinding, extraction, synthesis and filtration)	Leaves of plants with polyphenols Iron chloride (III) ($FeCl_3$) Deionized water Paper filters Energy	Solid waste Wastewater		Kuang et al. (2013); Martins et al. (2017); Joshi et al. (2018).

As an overview, for the nZVI synthesis through chemical methods, it is necessary to use chemical reagents such as iron chloride (III) ($FeCl_3$), sodium borohydride ($NaBH_4$), iron sulfate ($FeSO_4$), etc. in addition to argon, nitrogen, hydrogen. The use of these reagents results in environmental impacts due to their production, in addition to waste, wastewater and emissions that may contain some substance of these compounds. Thus, in relation to the inputs, the methods were classified with yellow and red colors. The latter is attributed to methods that involve the use of materials that can generate high risks to human health and the environment. According to GHS, these include sodium borohydride, isooctane and polyvinylpyrrolidone (PVP), and cetylpyridin chloride (CPC). The main aggravating factor in the use of chemical compounds is their ability to affect workers' health, in addition, these compounds are also distributed throughout the production processes, and may be in waste, wastewater and emissions generated.

Water consumption is low in most methods (i.e. up to 0.03 m^3 for production of 1.00 kg of nZVI). However, the ultrasonic wave method has a high rate of water consumption (above 0.071 m^3). The average consumption was verified in the liquid chemical reduction with the sodium borohydride, chemical gas reduction with hydrogen gas, electrochemical and green synthesis methods (from 0.031 to 0.07 m^3). Closely related to water consumption is wastewater generation through production methods; a direct relationship is perceived between these two aspects. In wastewater generation, the methods with higher amounts of water consumption are reduction with sodium borohydride, micro-emulsion and ultrasonic wave, while the methods with medium amounts are chemical gas reduction with hydrogen gas and green synthesis. The wastewater generated by the methods are composed of chemical components such as boron, chlorine, sodium, nitrate, sulfate, surfactants and stabilizers, these compounds give wastewater characteristics that make it dangerous to the environment and human health. Thus, all wastewater generated by the methods must undergo adequate treatment to meet the quality necessary for reuse or disposal.

According to the United Nations (UNESCO, 2020), in advanced economies, up to 45% of all water demand is generated by industry. As we move towards a future with more industrialized nations, this can have long-term consequences. In addition, with the growth of the overall demand for water, the amount of wastewater produced and its total pollution load are continuously increasing worldwide. More than 80% of the world's wastewater – and more than 95% in some less developed countries – is released into the environment without treatment (UN WWAP, 2017). Therefore, the industry must not only be more efficient with the water used, but also willing to explore the great possibilities offered by water reuse.

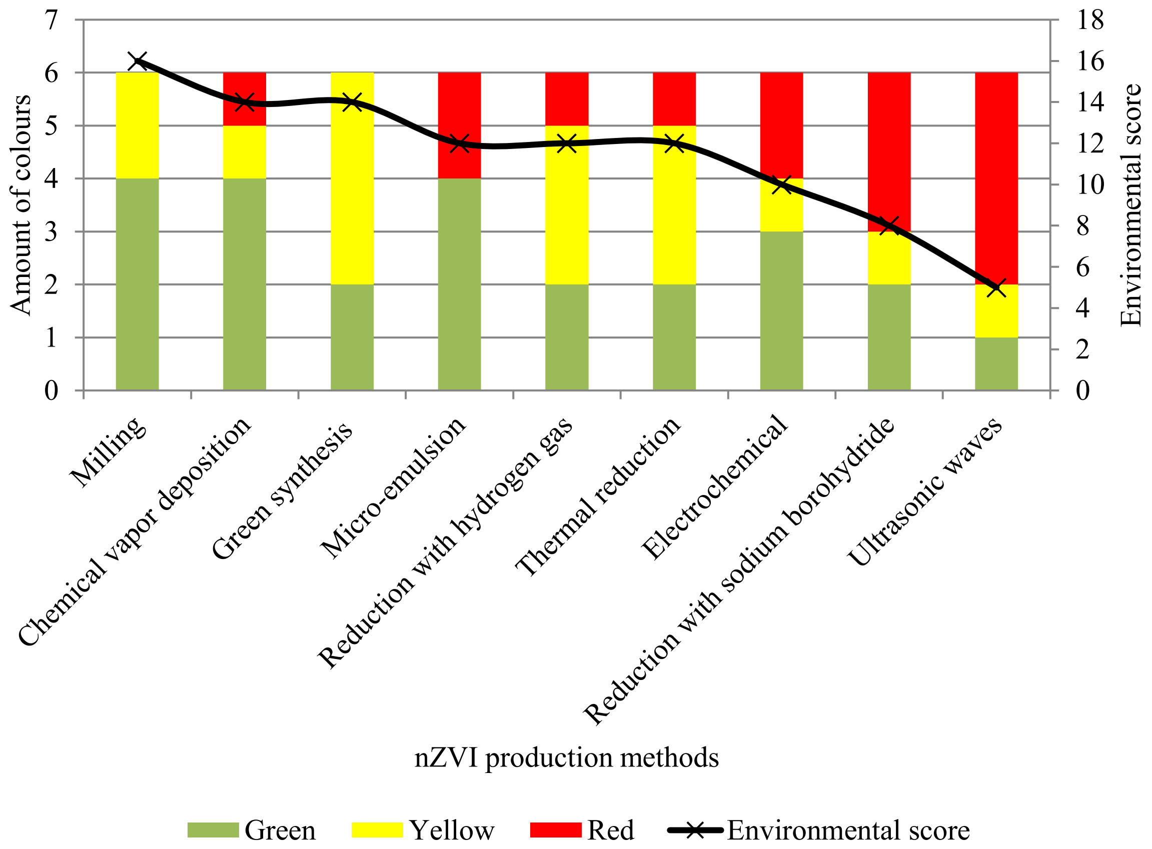
Energy consumption is an important factor in the methods' environmental aspects. It varies, with the highest consumption stemming from the methods of gas reduction with hydrogen gas and a medium-level in the ultrasonic wave method. High values of energy consumption in this study (above 61 kWh – corresponding to red on the scale) result in high environmental impacts. Energy consumption is related to environmental impacts of resource use (mainly in non-renewable energy matrices), gas emissions that affect human health and also that contribute to climate change. In addition, another factor that contributes to the environmental impacts of energy consumption is the energy matrix composition of the country where nZVI is produced. According to Visentin et al. (2019), in countries where the energy matrix is composed of non-renewable energies, the environmental impacts of nZVI synthesis may be greater. The environmental impacts of production are smaller in countries with an energy matrix with more renewable energy sources.

Solid waste generation occurs mainly in methods with a filtration process. In these methods, the filter used may contain some chemical compounds of the process reagents (i.e. boron, chlorine, sodium, nitrate, sulfate, surfactants and stabilizers), so it is necessary that an appropriate treatment process is carried out such incineration before the final destination. This classification includes methods such as sodium borohydride, thermal reduction, ultrasonic wave and green synthesis. However, the milling, chemical gas reduction with hydrogen gas, chemical vapor deposition, micro-emulsion and electrochemical methods do not generate residue during the process.

The last environmental aspect evaluated was atmospheric emissions. In this aspect, the methods that deserve to be highlighted are electrochemical, chemical vapor deposition and thermal reduction. In the electrochemical method, the generation of chlorine gas, which is toxic to people and the environment, occurs in the process. Thus, emission controls and handling measures are fundamental in this method. It is also worth mentioning the thermal reduction method that generates emissions such as monoxide and carbon dioxide. Furthermore, in the chemical vapor deposition method, gaseous carbonic compounds are formed, and in milling method, particulate matter with iron particles. It is necessary to have control measures and treatment of these emissions for synthesis of nZVI through these methods. These emissions contribute to impacts on the human health of workers and the community, as well as contributing to global warming.

A score was determined for each color on the color scale of environmental aspects classification in order to generate a final environmental score of the production methods. Thus, Figure II - 2 shows the total environmental score of each method and the quantification of the classification by color of each environmental aspect.

Figure II - 2: Environmental score of nZVI production methods.



The milling method resulted in the highest environmental score. In this method, it is perceived that the environmental aspects are classified mostly in green, with one in yellow. The materials used are corrosive and can cause irritation, and so are classified as yellow. However, water consumption, waste generation, waste water and emissions are minimal, which results in a better classification.

The chemical vapor deposition and green synthesis methods come in second in the ranking. The difference between these two methods is that the green synthesis method has only green and yellow aspects, while the chemical vapor deposition method has one aspect classified as red. The former method is considered an ecological method, but has four aspects classified as yellow due to inputs used. These are iron chlorite (III), water consumption, the solid waste and the wastewater generated. In the latter method, atmospheric emissions are classified as red.

The methods of reduction with hydrogen gas, thermal reduction and micro-emulsion are tied for third place in the ranking. The first two have the same number of aspects classified as green, yellow and red, while the third has more aspects classified as green and red, and none in yellow. In the hydrogen gas reduction method, energy consumption is responsible for the red color classification, while in the thermal reduction method, atmospheric emissions are. The micro emulsion method has two aspects classified as red: inputs and wastewater.

The three methods with the lowest rankings are electrochemical, reduction with sodium borohydride and ultrasonic wave. In these methods, there are fewer aspects classified as green and more as red. The electrochemical method has two aspects classified as red (inputs and atmospheric emissions), one as yellow and three as green, while the sodium borohydride reduction method has three aspects classified as red (inputs, solid waste and wastewater). The ultrasonic wave method has the lowest score of analyzed methods, with four aspects classified as red: inputs, water consumption, energy consumption and wastewater.

With this classification, the environmental behavior of nZVI production methods is generally perceived in relation to inputs, water and energy consumption, waste and wastewater generation, and emissions. Thus, it is possible to evaluate what measures are needed to improve the environmental aspects, as well as for practical use.

5 Advantages and disadvantages of nZVI production methods

Table II - 4 summarizes the main advantages and disadvantages of nZVI production methods, considering the characteristics of the nZVI produced and the production process, and also relating to environmental aspects.

Table II - 4: Advantages and disadvantages of nZVI production methods.

Methods	Advantages and disadvantages
Milling	*Advantages* • Simple method and equipment. • Easy operation. • It does not use toxic solvents. • It does not generate waste and wastewater. • nZVI produced is also reactive with contaminants. *Disadvantages* • High energy consumption. • Durability of milling equipment. • Difficulty in controlling the size and morphology distribution of NMs. • Strong tendency to agglomeration of the nZVI produced, due to very high surface energy.

Methods	Advantages and disadvantages
Liquid chemical reduction with sodium borohydride	*Advantages* • Simple and widely used method. • Simple laboratory equipment. *Disadvantages* • Use of expensive chemical reagents with high production impacts. • High tendency to particle agglomeration after production.
Gaseous chemical reduction with hydrogen gas	*Advantages* • Greater control of the nZVI characteristics. • Method applied on an industrial scale. *Disadvantages* • Complex method with many production steps. • High energy consumption. • High costs.
Thermal reduction	*Advantages* • Simple and inexpensive method, easy operation. • Production of nZVI encapsulated by carbon (C-Fe0), resulting in a lower aggregation of particles. • Use of simpler carbon-based materials such as black carbon and biochar. • Generation of waste and effluents with lower concentration of chemicals (simpler treatment). *Disadvantages* • CO, CO_2 emission. • Energy consumption.
Chemical vapor deposition	*Advantages* • *G*reater control over the characteristics of the NPs produced. • Smaller agglomeration of NPs. *Disadvantages* • High production cost. • The process generates by-products, which must be removed by a continuous flow of gas. • Poorly studied method for the nZVI production.
Micro-emulsion	*Advantages* • *C*ontrol over the size and morphology of NPs. • Low power consumption. • Use of simple equipment. *Disadvantages* • Generation of waste and wastewater with high concentrations of oils, surfactants, surfactants and chemicals. • High oil consumption and surfactants • High costs, especially with surfactants. • Low production quantity.
Ultrasonic waves	*Advantages* • Uniform particles with greater control of morphology and size. • Ease of deployment. • Requires simple and inexpensive equipment. *Disadvantages* • High production costs due to reagents. • Adequate treatment is required for waste wastewater generated.

Methods	Advantages and disadvantages
Electrochemical	*Advantages*
	• Use of simple and inexpensive reagents. • Ease of assembly and operation, requires simple equipment.
	Disadvantages
	• The process generates chlorine gas, which should be more careful due to the dangers of exposure to process operators, using appropriate protective equipment, when in contact with human airways, chlorine gas can generate irritations and inflammation.
Green synthesis (with plant extracts)	*Advantages*
	• Eco friendly method. Simple and inexpensive method. • Low costs (green synthesis with plant extract). • Lower toxicity of the reducing agent used compared to sodium boron hydride. • Low power consumption. • Waste and wastewater generated with less toxicity. • Increased reactivity in nZVI particles. • Valuing the use of natural products.
	Disadvantages
	• In the green synthesis using plant extract occurs the destruction of these plants. • In this process, incomplete Fe reduction occurs. • Less control over the size and morphology of NPs. • Agglomeration of NPs. • In the process of synthesis of microbial reduction is necessary aseptic conditions, which requires trained personnel, increasing production costs.

In general, all methods result in advantages and disadvantages related to the characteristics of the production process in terms of production stages, equipment used and quantity of inputs, as well as in the generation of waste, wastewater and emissions, and in the high consumption of water and energy.

According to Crane and Scott (2012) the methods of reduction with sodium borohydride, reduction with hydrogen gas, chemical vapor deposition, microemulsion and ultrasonic waves result in highly reactive nZVI, however, nanoparticles are often highly polydispersed, ranging from tens to hundreds of nanometers in size and therefore significantly subject to agglomeration. In the method of thermal reduction and reduction with hydrogen gas the nZVI produced is already stabilized during production, minimizing the agglomeration of particles.

Another disadvantage of the methods is the use of expensive reagents and also in high quantities, such as iron acetate and sodium borohydride (Crane and Scott, 2012; Visentin et al. 2019). In addition, due to the high amount of inputs, waste and wastewater generated, it preclude the industrial application of methods such as reduction with sodium borohydride, micro-emulsion, ultrasonic waves and electrochemical.

Visentin et al. (2021) demonstrates that the reduction with sodium borohydride method results in high environmental impacts, while the reduction with hydrogen gas method has high production costs. Moreover, the production of nZVI by milling method is sustainable. Martins et al. (2017) demonstrate that the green synthesis method results in lower life-cycle environmental impacts and costs than the sodium borohydride reduction method.

6 Conclusion

There are numerous methods that can be used in nZVI synthesis. They differ mainly according to the technology employed (from top-down or bottom-up) and the production mechanism (physical or chemical), in addition to specific characteristics of the method and the nZVI produced.

Nine production methods are listed, according to a survey from the worldwide computer network and scientific databases. Six methods (67%) apply to laboratory-scale studies and three (33%) are used by industries (milling, gas reduction and chemical vapor deposition). However, many of the companies that sell nZVI do not disclose the method employed in production.

Regarding production methods, only one comprises a top-down technology (milling). The most popular method in scientific papers is chemical reduction with sodium borohydride as a reducing agent, and also thermal reduction. Green synthesis is a method that has been becoming more popular in laboratory studies and applications, mainly because it is seen as eco-friendly. The methods of ultrasonic wave, electrochemical and thermal reduction are the most recent, and their application occurs on a laboratory scale, but can be easily applied in industrial productions. The micro-emulsion method can be used both in nZVI production and in improving its characteristics. The method of chemical vapor deposition is one with the smallest studies published in the databases, mainly due to its lower utilization because of high production costs.

An environmental criteria classification of the methods was proposed to demonstrate, through a semi-qualitative evaluation with a color scale and score, the environmental behavior of the methods in relation to inputs, water and energy consumption, waste generation, wastewater generation and atmospheric emissions. It was noticed that in general, all methods generate solid waste, wastewater and atmospheric emissions throughout their production. These generated by-products should be treated appropriately, as many may contain chemicals harmful to the environment and the population. In addition, many of the methods result in high energy and resource consumption, and consequently high production costs.

Through a score established for each color scale classification, it was possible to determine an environmental ranking of the methods. Thus, the milling method was classified as the best, followed green synthesis and chemical vapor deposition. The methods with the lowest scores were ultrasonic wave, reduction with sodium borohydride and electrochemical. This type of classification is simple and demonstrates the general environmental behavior of the methods. In addition, this analysis is the initial step towards attaining more detailed knowledge about the methods' environmental aspects and carrying out studies on their sustainable aspects.

From this study, there are opportunities for future work, such as: (1) determining weighting factor for the color scale of classification of each environmental aspect; (2) quantitative analysis of the environmental impacts of nZVI production methods, and (3) analysis of the social and economic aspects of the methods, in order to obtain an assessment of sustainability.

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Supplementary Material

Table 1A. Life cycle inventory of nZVI production methods

Methods	Life cycle inventory	
	Inputs/Outputs	Amount
Milling	Iron particles	1.00 – 3.00 kg
	Energy	30 – 50 kWh
	Atmospheric emissions	1.00×10^{-4} - 2.00×10^{-4} g
Liquid chemical reduction with sodium borohydride	Iron chloride (III) ($FeCl_3$)	3.0 – 5.0 kg
	Sodium borohydride ($NaBH_4$)	2.0 – 4.0 kg
	Deionized water	0.05 - 0.1 m^3
	Ethanol	2.0 – 4.0 kg
	Energy	0.05 – 0.5 kWh
	Paper filters	2.0 – 3.0 kg
	Wastewater	0.07 – 0.1 m^3
	Solid waste	2.5 – 3.0 kg
Gaseous chemical reduction with hydrogen gas	Sodium carbonate ($NaCO_3$)	2.0 - 4.0 kg
	Iron Sulfate (II) ($FeSO_4$)	2.0 – 3.0 kg
	Nitrogen (N_2) (gas)	2.0 – 3.0 kg
	Iron carbonate ($FeCO_3$)	2.0 – 4.0 kg
	Aluminum hydroxide $Al(OH_3)$	0.1 – 0.3 kg
	Energy	100 – 120 kWh
	Gaseous hydrogen (H_2)	0.03 - 0.05 kg
	Deionized water	0.02 - 0.03 m^3
	Wastewater	0.03 – 0.05 m^3
Thermal reduction	Iron nitrate (III) $Fe(NO_3)$	1.0 - 3.0 kg
	Carbon black	0.2 - 0.4 kg
	Deionized water	0.01 - 0.02 m^2
	Nylon membrane	0.1 - 0.2 kg
	Iron(III) Acetate $(C_2H_3O_2)_3$	3.0 – 5.0 kg
	Argon	0.05 - 0.08 kg
	Energy	30 – 40 kWh
	Wastewater	0.01 - 0.02 m^3
	Solid waste	1.0 – 3.0 kg
	Atmospheric emissions	0.1 - 0.2 m^3
Chemical vapor deposition	Iron pentacarbonyl ($Fe(CO)_5$)	2.0 - 4.0 kg
	Ethyl (C_2H_5)	0.02 - 0.04 kg
	Ethylene (C_2H_4)	0.01 - 0.02 kg
	Acetylene (C_2H_2)	0.04 - 0.06 kg
	Argon	7.0 - 9.0 kg
	Energy	1.0 – 5.0 kWh
	Atmospheric emissions	8.0 - 10 kg
Micro-emulsion	Iron Sulfate (II) ($FeSO_4$)	2.0 - 3.0 kg
	Borohydride potassium (KBH_4)	1.0 – 2.0 kg
	Surfactant	170.0 - 180.0 kg
	n-butanol	80.0 - 90.0 kg
	Isooctane	350.0 - 360.0 kg
	Deionized water	0.01 - 0.03 m^3
	Anhydrous ethanol	0.002 - 0.004 m^3
	Acetone	0.002 - 0.004 m^3
	Argon	0.01 - 0.02 kg
	Energy	1.0 – 5.0 kWh

	Solid waste	0.01 - 0.02 kg
	Wastewater	0.8 – 1.0 m³
Ultrasonic waves	Iron Sulfate (II) ($FeSO_4$)	4.0 - 6.0 kg
	Sodium borohydride ($NaBH_4$)	1.5 – 3.0 kg
	Ethanol	0.3 – 0.5 m³
	Nitrogen	0.3 - 0.6 kg
	Deionized water	0.1 - 0.3 m³
	Nylon filter membrane	0.5 - 0.6 kg
	Energy	61 – 70 kWh
	Wastewater	0.1 – 0.3 m³
	Solid waste	0.5 - 0.6 kg
	Atmospheric emission	0.2 - 0.3 kg
Electrochemical	Iron chloride (III) ($FeCl_3$)	2.0 – 3.0 kg
	Deionized water	0.01 – 0.03 m³
	Stabilizers (e.g., polyvinylpyrrolidone (PVP), cetylpyridin chloride (CPC))	2.0 – 4.0 kg
	Argon	0.01 – 0.02 kg
	Energy	0.05 – 0.5 kWh
	Wastewater	0.01 – 0.03 m³
	Atmospheric emissions	0.7 - 0.8 kg
Green synthesis (with plant extracts)	Leaves of plants with polyphenols	2.0 – 3.0 kg
	Iron chloride (III) ($FeCl_3$)	3.0 – 4.0 kg
	Deionized water	0.03 - 0.06 m³
	Paper filters	2.0 – 3.0 kg
	Energy	0.1 – 0.5 kWh
	Solid waste	0.05 – 1.0 kg
	Wastewater	0.03 - 0.04 m³

4 CAPÍTULO III (artigo de resultados – publicado): Sustainability assessment of nanoscale zero-valent iron production methods[3]

Abstract: Nanoscale zero-valent iron (nZVI) is the main nanomaterial used in remediation processes. The aim of this study was to evaluate the sustainability of the nZVI production methods. For this, nine nZVI production methods were selected for analysis. Four kinds of life cycle analysis were performed: life cycle assessment (LCA), life cycle cost (LCC), social life cycle assessment (S-LCA), and life cycle sustainability assessment (LCSA). LCA was performed in the SimaPro® program using the Impact 2002+ method. LCC was also done in SimaPro® by developing a cost analysis method. For the social analysis, equations were used to calculate the social life cycle score. For LCSA, the results of the life cycle analyses were normalized, and a weighting factor was defined on the basis of multi-criteria analysis methods. The sustainability score was calculated on the basis of a linear additive model. Scenario and sensitivity analyses were performed, and Monte Carlo simulation was used to quantify the uncertainty of the results. The system limits system includes the stages of raw material extraction, transportation, and nZVI production. The functional unit was 1.00 kg of nZVI produced. The green synthesis method was found to be the most sustainable method, classified as highly sustainable, while the micro-emulsion method was found to be the least sustainable method, classified as unsustainable. The scenario analysis showed that overall, the Swiss and Canadian scenarios have the highest sustainability index scores while the Indian scenario has the lowest. In addition, the results show low sensitivity to weighting factor variation. In general, this study contributed to the state-of-the-art LCSA application on nanomaterials used in remediation.

Keywords: Sustainable remediation; soil remediation; environmental impacts; environmental costs; social index.

1 Introduction

To understand and optimize the impact of a product throughout its life cycle, the consideration of its environmental, economic, and social factors is of increasing interest

[3] *VISENTIN, C.; BRAUN, A. B.; TRENTIN, A. da S., THOMÉ, A. Sustainability Assessment of Nanoscale Zerovalent Iron Production Methods.* ***Environmental Engineering Science****, v. 39, n. 10, p. 847-860, 2022. https://doi.org/10.1089/ees.2021.0341*

to decision makers and regulatory institutions (Riedelsheimer et al. 2020). As such, life cycle sustainability assessment (LCSA), a tool used to evaluate and understand the trade-offs of the three dimensions of sustainability from the point of view of the life cycle, has received increasing attention over the years (Costa et al. 2019; Riedelsheimer et al. 2020; Visentin et al. 2020; Alejandrino et al. 2021).

LCSA emerged from the need to incorporate the three pillars of sustainable development into a single formulation, maintaining the perspective of the life cycle (Fauzi et al., 2019; Visentin et al. 2020). Thus, the traditional life cycle assessment (LCA) method was expanded to include economic and social analyses (van Kempen et al., 2017). Unlike the traditional sustainability assessment tools, LCSA can identify the sustainability of a product from a life cycle perspective (Ren et al., 2015). According to Klöpffer (2008), LCSA results in LCA integration, life cycle cost (LCC), and social life cycle assessment (S-LCA).

Nanoscale zero-valent iron (nZVI) is the most widely used nanomaterial in the United States and Europe for soil and groundwater remediation (Grieger et al. 2019; Liu et al. 2021). It is popular because it is considered a potentially cost-effective alternative to the conventional treatment technologies (e.g., reactive barriers and pump and treat), which often require more time and intensive resources (Grieger et al. 2019; Li et al. 2021). In addition, nZVI can be applied in the remediation of numerous contaminants, both organic and inorganic compounds such as heavy and radioactive metals (Chen et al. 2019; Cecchin et al. 2021).

Nanomaterials can be produced in several ways, but two technologies have been highlighted: manufacturing through the top-down and bottom-up processes (Thomé et al. 2015). The top-down processes are usually physical synthesis methods involving the use of particles larger than nanometric as powder or bulk elements; during synthesis, the elements become nanometric in size Visentin et al. (2021b). The bottom-up methods are the opposite; they start from materials smaller than nanometric, such as atoms and molecules, which through chemical processes go beyond nanometric in size. Regarding nZVI, nine production methods were reported by Visentin et al. (2021b): milling, liquid chemical reduction with sodium borohydride, gaseous chemical reduction with hydrogen gas, thermal reduction, chemical vapor deposition, microemulsion, ultrasonic wave method, electrochemical method, and green synthesis.

Over the past few decades, there has been a gradual increase in the concern about the sustainability of soil and groundwater remediation processes due to the concern about the impacts and benefits of remediation (Braun et al. 2019). The dissemination of sustainable remediation has expanded the concern regarding remediation processes beyond decontamination. This approach is broader and considers the environmental, economic, and social impacts of the life cycles of remediation processes (Rizzo et al. 2016; Braun et al. 2019). As such, methods and tools that can help decision makers in selecting the remediation technique to employ from among the existing techniques on the basis of the results of the analysis of their impacts have been developed. Among such tools are life cycle analysis methods such as LCA, LCC, S-LCA, and LCSA (Visentin et al. 2019; Jin et al. 2021; Visentin et al. 2021a).

Despite the numerous benefits of using nZVI in remediation, there are still many uncertainties regarding such and many research gaps about it to be filled, such as in relation to the long-term behavior in the soil, toxicity, and the environmental, economic, and social impacts of the nZVI production methods (Shafi et al. 2021). The scientific community is particularly interested in evaluating the impacts of nZVI production, as shown by the studies of Martins et al. (2017), Joshi et al. (2018), and Visentin et al. (2019; 2021a; 2021c). Martins et al. (2017) evaluated the environmental impacts and costs of chemical reduction with sodium borohydride and green synthesis through production from plant extracts. In this study, the green synthesis method resulted in the lowest environmental impacts and costs (Martins et al. 2017). Johsi et al. (2018) analyzed the environmental impacts of the green synthesis method with the microbial reduction of natural Fe (III). In which it found that the environmental impact hotspots are raw material resourcing, followed by natural gas and electricity consumptions (Joshi et al. 2018). The methods of milling, reduction with sodium borohydride, and reduction with hydrogen gas were evaluated the environmental impacts and costs in Visentin et al. (2019b) and the social impacts in Visentin et al. (2021c). However, these studies evaluated only the environmental and economic aspects of nZVI production rather than sustainability as a whole. To date, there has been one study (i.e., Visentin et al. 2021a) that focused on the analysis of the life cycle sustainability of three nZVI production methods: milling, reduction with sodium borohydride, and reduction with hydrogen gas. However, according to Visentin et al. (2021b), there are nine nZVI production methods.

This research intends to contribute to the scientific community on the subject studied, since it is the first study that comprehensively evaluates the sustainability of all nZVI production methods. The new contributions of the present study are: (i) assess the environmental, economic and social life cycle impacts of nine nZVI production methods; (ii) determine the sustainability of the production methods of the nZVI; (iii) perform scenario, sensitivity and uncertainty analysis in the LCSA results; and (iv) verify the variability of LCSA results considering the stakeholders participation.

Thus, this study aimed to evaluate the sustainability of nine nZVI production methods, through a life cycle analysis tools. To this end, some specific objectives were outlined: (a) to perform environmental (LCA), economic (LCC) and social (S-LCA) life cycle analysis in the nine nZVI production methods cited by Visentin et al. (2021b); (b) to perform a LCSA of production methods through multi-criteria analysis methods, AHP, and expert participation; (c) to determine which nZVI production method is the most sustainable; and (d) to verify the variability of the LCSA results through analysis of scenarios, sensitivity and Monte Carlo.

2 nZVI production methods

Nanomaterials can be produced in several ways, but two technologies have been highlighted: manufacturing through the top-down and bottom-up processes (Thomé et al. 2015). The top-down processes are based on larger materials such as particles and bulk materials, which undergo certain processes, usually physical, to decrease their sizes to nanometers. The bottom-up processes, on the other hand, start from materials smaller than nanometric, such as atoms and molecules, which, through chemical processes for example, are transformed and become nanometric in size (Thomé et al 2015; Visentin et al. 2021b).

For the nanomaterial nZVI, its existing production methods are milling, liquid chemical reduction with sodium borohydride, gaseous chemical reduction with hydrogen gas, thermal reduction, chemical vapor deposition, microemulsion, ultrasonic wave method, electrochemical method, and green synthesis (Visentin et al. 2021b). Table III - 1 shows the production mode of all these nZVI production methods, the characteristics of the nZVI produced. The production flowcharts with all the inputs and outputs of each production stage are presented in the Supplementary Material.

Table III - 1: nZVI production methods – production process, characteristics of the nZVI produced.

Methods	Description
Milling	Iron particles are inserted into a rotating chamber together with steel spheres (250 µm in diameter), which consist of the nZVI formation medium. Through the equipment rotation, the iron particles are crushed by the steel spheres, and the impact energy breaks the iron particles into smaller pieces until it reaches the size of nanometer. The operation of the equipment is eight hours for an nZVI size of 20 nm. *Diameter:* 10 - 50 nm *Specific surface area:* 39.0 m²/g *Production scale:* Laboratory and industrial References: Li et al. (2009); Jung et al. (2015); Visentin et al. (2019).
Chemical reduction with sodium borohydride	The synthesis process occurs by mixing equal volumes of aqueous solutions of sodium boron hydride ($NaBH_4$) and iron chloride ($FeCl_3$). The mixtures of the solution are stirred continuously (about twenty minutes). After the synthesis reaction, nZVI goes through the processes of washing, filtering and drying. Washing is performed with deionized water, ethanol or acetone and drying under inert atmosphere. Washing with ethanol and acetone is used to prevent immediate oxidation of nZVI during purification (Martins et al. 2017; Visentin et al. 2019). *Diameter:* 1 - 100 nm *Specific surface area:* 30.0 m²/g *Production scale:* Laboratory References: Barreto-Rodrigues et al. (2017); Martins et al. (2017); Visentin et al. (2019).
Chemical reduction with hydrogen gas	The production of nZVI by this method initially involves the production of goethite and hematite particles through inert atmosphere reduction processes. The goethite and hematite particles produced are reduced by heat to a temperature of 350 to 600 ° C in a hydrogen gas atmosphere. After synthesis, nZVI particles are oxidized in water and then dried in a kiln. *Diameter:* 40 - 70 nm *Specific surface area:* 29.0 m²/g *Production scale:* Industrial References: Uegami et al. (2009); Visentin et al. (2019).
Thermal reduction	Iron oxide particles or iron salts are hydrated and reduced at high temperatures (above 500°C), with the use of thermal energy, in N_2 atmospheric with the presence of gaseous reducing agents such as H_2, CO_2 or CO produced along the thermal decomposition of carbon-based materials (black carbon, biochar, carbon nanoparticles). *Diameter:* 20 - 150 nm *Specific surface area:* 130.0 m²/g *Production scale:* Laboratory References: Hoch et al. (2008); Dai et al. (2016); Stefaniuk et al. (2016); Orlandi et al. (2017).
Chemical vapor deposition	The chemical vapor deposition method consists of a vaporization process, in which the target materials are initially vaporized by heat sources for after being quickly condensed. The reagents (precursor material, reducing agent and gas) are inserted into the reaction chamber. This chamber is heated, and for a short period (10 minutes) occurs to the synthesis reaction, forming the nZVI. The nanoparticles condense into a rotating liquid nitrogen substrate and are transferred to the delivery system, in which they can be scraped and collected. *Diameter:* 25 nm *Specific surface area:* 40 - 60 m²/g *Production scale:* Laboratory and industrial References: Park and Sudarshan (2001); Tavakoli et al. (2007).

Methods	Description
Micro emulsion	Mixture of microemulsions, one containing the metal precursor (iron chloride) and the other containing the precipitating agent (sodium borohydride). After mixing, both reagents will come into contact with each other due to droplet and coalescence collisions, and react to form precipitates of nanometric size. Nucleation and growth reactions occur within the droplets, which control the final size of the particles After this process occurs again a agitation, and then the material is centrifuged in order to separate the particles, and after they are washed with ethanol or acetone and then removed. *Diameter:* 40 - 60 nm *Specific surface area:* 140 - 160 m²/g *Production scale:* Laboratory References: Li et al. (2003); Capek (2004); Sanchez-Dominguez et al. (2012).
Ultrasonic waves	Synthesis is performed in a balloon reactor with three open necks. Initially, Fe^{+3}, $NaBH_4$ and ammonium hydroxide solutions are prepared with deionized water. Ultrasound is applied by means of a titanium probe submerged in the solution, with a constant frequency. Nitrogen gas is injected into the other necks of the vial in order to remove oxygen and prevent oxidation in the process. The reaction balloon is submerged in water to maintain the solution temperature. The solid produced in the reaction (Fe^0) should be filtered, washed (ethanol or acetone) and dried (in a kiln or vacuum oven). *Diameter:* 10 nm *Specific surface area:* 34.0 - 42.0 m²/g *Production scale:* Laboratory References: Jamei et al. (2014); Stefaniuk, et al. (2016).
Eletrochemical	The production of nZVI occurs initially by the preparation of iron chloride solution. Production takes place in an electroplating reactor, inside an ultrasonic vibrator (with water inside), which aid removal in the nZVI before grouping, and are used simultaneously during the reaction to provide physical energy for nZVI removal. The nZVI produced should be collected under oxygen-free water. Stabilizers are firmed to prevent the grouping of the nZVI particles produced. *Diameter:* 1 - 20 nm *Specific surface area:* 25.4 m²/g *Production scale*: Laboratory References: Chen et al. (2004)
Green synthesis	May occur through plant extracts and microorganisms. Green synthesis with plant extracts occurs mainly with those with high polyphenol indexes, and high antioxidant capacity, such as plants such as coffee, green tea, black tea, lemon, balm, bran, grape, etc. The production takes place through the preparation of the polyphenolic solution, by heating plant extracts in water, to a temperature close to the boiling point. After the separation of the plant residue extract occurs through filtration. After the extracts are mixed with a solution of Fe^{3+}. Iron ions in the presence of polyphenols are reduced to Fe^0. *Diameter*: 20 - 120 nm *Specific surface area:* 5.8 m²/g *Production scale:* Laboratory References: Machado et al. (2013); Stefaniuk et al. (2016); Martins et al. (2017)

3 Methodology

The four kinds of life cycle analysis that were performed (LCA, LCC, S-LCA, and LCSA) were based on the ISO 14040 (2006) steps.

The analyses were performed for the nine nZVI production methods (milling, reduction with sodium borohydride, reduction with hydrogen gas, thermal reduction, chemical vapor deposition, microemulsion, ultrasonic wave method, electrochemical method, and green synthesis) according to the study by Visentin et al. (2021b).

The goal of life cycle analysis in this study was to evaluate the environmental, economic, social impacts and the sustainability of the life cycles of the nine nZVI production methods. All life cycle analyses have the same system boundary and functional unit, to allow for an adequate comparison between the different methods, according to ISO 14040 (2006) methodology. The system boundary involves the cradle-to-gate approach, i.e., it considers the steps of raw-material extraction to nZVI production, not being considered the use stage. The functional unit that was used was 1.00 kg of nZVI produced by each method. Previous studies evaluating the life cycle impacts of nZVI production methods also used functional units of mass unit, being 1.00 kg (Joshi et al. 2018) and 1.00 g (Martins et al. 2017). For this study it was considered that all the nZVI have the same efficiencies, this being in the range of 60 to 99% (Dai et al. 2016; Barreto-Rodrigues et al. 2017; Cecchin et al. 2021; Liu et al. 2021).

3.1 Life cycle analysis (LCA, LCC and S-LCA)

- **Inventory analysis**

Inventory data were collected using secondary data. Primary data were not used as their collection would have been hampered by the privacy policies of the companies that produce nZVI. Thus, all the inventory data were secondarily obtained from publications (as can be seen in Table III-1), from estimates, from databases such as ecoinvent, and from worldwide reports. The data quality of the life cycles comprises the scan coverage, geographic coverage, accuracy, relevance, completeness, validity, and consistency. The ecoinvent data that were used were from the latest available version of the database (version 3.6, 2019). Data were selected from the database considering the allocation model at the point of substitution (APOS) (Ekvall, 2019) and the geographical location Rest-of-the-World (RoW). In the social analysis, the data of the social indicators were at the country level.

The economic indicators that were used corresponded to the internal and external costs of the nZVI production method life cycle. The internal costs were the direct production costs, such as the costs for the acquisition of raw materials and reagents, the energy costs, the labor costs, and the costs of incineration of industrial solid waste and treatment of industrial wastewater. The cost of infrastructure (building construction, utility costs of operating building) and taxes was not included. The external costs, on the other hand, were the environmental costs. These costs were related to the impact categories of LCA, such as: acidification, eutrophication, toxicity, global warming, ozone layer depletion, photochemical oxidation, and inorganic respiratory emission.

Table 2a of Supplementary Material presents the environmental and economic inventory data of the nine production methods of nZVI. All the data were based on the functional unit of life of 1.00 kg of the nZVI produced. The operational details of the methods regarding the equipment used, power, and equipment operation time can be checked in the Supplementary Material.

In S-LCA, the data collection was structured through a set of indicators associated with the impact categories and stakeholders. These indicators were determined prior to the application of S-LCA through a systematic review in the publications referring to such method. Thus, four categories of stakeholders (workers, local community, society, and value chain), 14 impact categories, and 34 indicators were selected. Table 3a of Supplementary Material presents the impact categories and social indicators.

- **Impact assessment**

In this work, an attributional LCA method was performed in the SimaPro® program (version 9.1) using the Impact 2002+ method, that was chosen because it is used in numerous studies of LCA with nanomaterials, and also because this method has already been used by authors in previous published studies that complement this work.

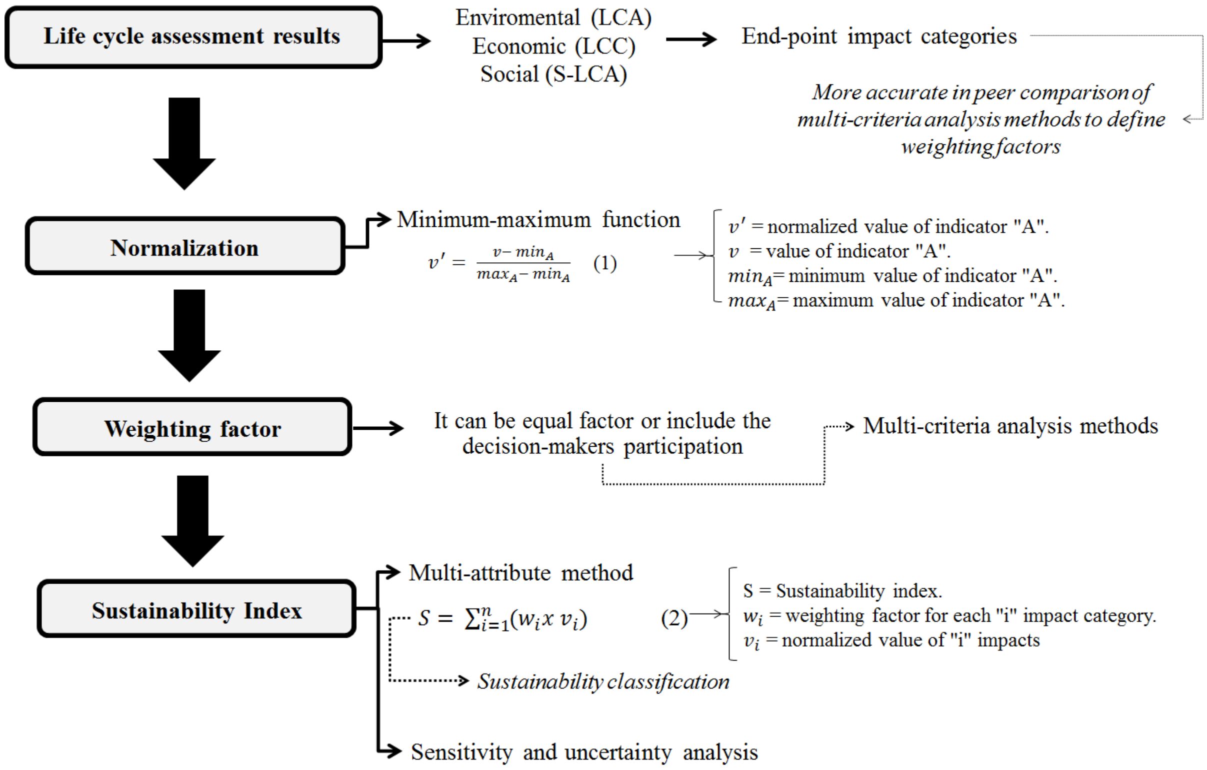
LCC was performed in SimaPro® by developing a cost analysis method using the method of Visentin et al. (2019b; 2021a). To reduce the uncertainty of the LCC results, Monte Carlo simulation was performed. The initial costs (external and internal) resulting from the application of LCC was analyzed through 10,000-time total Monte Carlo simulation, with 0.80 probability (p-value). In this type of study, it is very difficult to have accurate estimated costs, so the p-value was set at 0.80 (Wang, Chang and El-Sheikh, 2012; Visentin et al. 2021a). After the application of the method, the average of the values obtained from the attempts was set as the life cycle cost value. The final life cycle costs are presented herein in U.S. dollars (US$).

In the S-LCA, the social impacts were analyzed using the method of Hossain et al. (2018) and Visentin et al. (2021c). This methodology is based on equations to determine the impacts of midpoint and end point in the categories of stakeholders considered. Initially, social inventory data should be normalized for common units using the minimum-maximum equation. After equations are applied (check in supplementary material) that relate the normalized score of social indicators with weighting factors for the calculation of the impacts of point method and end point. Finally, a social life cycle score is calculated. The methodological procedure for calculating the impacts of S-LCA is detailed in the Supplementary Material. All social life cycle score calculations were carried out in Excel. The social life cycle score is an adimensional index of values from 0.00 to 1.00; the closer the index is to 1.00 the more socially positive it is.

3.2 Life cycle sustainability assessment

The LCSA was based on the results of the life cycle analyses (LCA, LCC, and S-LCA) in the endpoint impact categories, according to Visentin et al. (2021a). For this, comparison of pairs for multi-criteria analysis was favored, yielding more accurate results than the comparison of the environmental, economic, and social aspects of the nZVI production methods. In LCA the end-point impact categories were selected because they facilitate in the process of analyzing the AHP method. While using the midpoint impact categories there would be more variables to be analyzed, which could increase the respondent's difficulty and also the consistency of the results. Figure III – 1 summarized LCSA methodology.

Figure III - 1: Life cycle sustainability assessment methodology.



The results of the life cycle analyses in the endpoint categories were normalized in a common unit using the minimum–maximum normalization function, according to Visentin et al. (2021a) and to Equation 01 of Figure III - 1. The normalized values range from 0.00 to 1.00, where 0.00 corresponds to more negative impacts while 1.00 corresponds to more positive impacts.

In LCSA, sustainability is determined through sustainability index. For the calculation of the sustainability index, the weighting factors for the sustainability analysis must be defined. This factor can have equal values for all the impact subcategories (respecting the rule that the sum of the weighting factors must be equal to 1.00) or it can be a value defined by experts using multi-criteria analysis methods for example, such as the analytical hierarchical process (AHP) (Visentin et al. 2021a). The weighting factors that were used in this study were those defined by Visentin et al. (2021a) in the endpoint impact categories. Table 4a of Supplementary Material presents the weighting factors for the sustainability index score calculation

With the normalized values of the impacts and weighting factors, the multi-attribute value method, in which the sustainability index score is calculated (Equation 02 of Figure 1), is applied. The sustainability is classified according to the classification system defined by Hossain et al. (2018): Highly unsustainable (0.00 – 0.20);

Unsustainable (0.21 – 0.40); Neutral (0.41 – 0.60); Sustainable (0.61 – 0.80); and Highly Sustainable (0.81 – 1.00).

3.2.1 Complementary analyses

Complementary analyses were performed to evaluate the sensitivity and uncertainty of the LCSA results. Thus, scenario, sensitivity and uncertainties were performed.

3.2.1.1 Scenario analysis

Scenario analysis was performed in the life cycle analyses (LCA, LCC, and S-LCA). This analysis was based on the variation of the data location scenarios. For each life cycle analysis different variations were carried out:

- LCA, only the energy data for all the methods were varied. For all the nZVI production methods, the energy data were selected considering the location of the data for the U.S. scenario. In the sensitivity analysis, how the data could be affected by the changes in the location of the electricity data and in the compositions of the energy matrices of the different countries was evaluated.
- LCC was performed while simultaneously varying (i) the cost of the industrial energy applied by the different countries studied; (ii) the external environmental costs, basis of the LCA scenario analysis results, and (iii) labor costs of each country.
- S-LCA was performed while simultaneously varying (a) the data on the indicators of the different countries studied and (b) the environmental behaviors of the nZVI production methods based on the results of the LCA sensitivity analysis.

Thus, 10 scenarios were considered for this analysis, selected according to different criteria, such as the world's large economies, the social progress index, the global sustainability index, the environmental performance index, the countries with a higher renewable-energy share in their energy matrices, the countries that had published the most about "soil remediation" (Scopus and Web of Science), and the countries with nZVI production companies. The 10 countries that were selected on the basis of these criteria were Brazil, Canada, China, the Czech Republic, Germany, India, Japan, Switzerland, the UK, and the U.S.

3.2.1.2 Sensitivity analysis

Sensitivity analysis was performed by varying the weighting factors of the impact categories. These weights were determined through multi-criteria analysis using the AHP method (as per the previous item). Three weighting factor variations were performed: (1) equal weights for all the impact categories; (2) experts' preference for the environmental, economic, and social aspects; and (3) application of a single range of weight deviations (± 20%) for all the impact categories relative to their current weights.

In the analysis with equal weights, a 0.11 weight was used for all the impact categories. In the analysis of the experts' preference for the environmental, economic, and social aspects, three scenarios were analyzed: (1) one where the experts gave the environmental aspect a 50% weight preference (economic aspect, 25%; social aspect, 25%); (2) one where the experts gave the economic aspect a 50% weight preference (environmental aspect, 25%; social aspect, 25%); and (3) one where the experts gave the social aspect a 50% weight preference (environmental aspect, 25%; economic aspect, 25%).

The third variation was performed through the one-at-a-time approach, in which the weights of the impact categories were changed one at a time and the effect on the final result was verified (Rizzo et al. 2016; Visentin et al. 2021a). Increments were applied for each impact category, and the weights of the other impact categories were adjusted proportionally (± 2.5%) so that the sum of the weights would be equal to 1.00.

3.2.2 Uncertainty analysis

To reduce the uncertainties of the LCSA results, Monte Carlo simulation was performed. For this study, a discrete distribution of probabilities was used. This analysis was performed in Microsoft Excel. The sustainability index values obtained from the LCSA were analyzed through 10,000-time total Monte Carlo simulation, with 0.95 probability (p-value). Nine Monte Carlo simulations were performed with the sustainability index results of each nZVI production method.

4 Results and Discussion

4.1 Life cycle analysis (LCA, LCC and S-LCA)

The results of the environmental, economic, and social life cycle analyses are presented in Table III - 2. The environmental impacts of LCA are expressed in mPt (millionth of points), the life cycle costs are expressed in U$/kg, and the social impacts are expressed through scores from 0.00 to 1.00, with 1.00 representing a method with better social indices, and have no unit.

Table III - 2: Results of the life cycle analyses (LCA, LCC and S-LCA).

Life cycle	Impacts	Life cycle results								
		Milling	Reduction with sodium	Reduction with hydrogen gas	Thermal reduction	Chemical vapor deposition	Micro-emulsion	Ultrasonic wave	Eletrochemical	Green synthesis
LCA	Human Health (mPt)	5.30	22.80	17.41	7.49	4.26	352.28	77.22	1.96	1.07
	Quality of Ecosystems (mPt)	0.47	13.39	1.62	1.08	0.77	482.61	66.52	0.43	6.93
	Climate Change (mPt)	2.01	8.72	6.85	3.94	2.23	261.04	8.48	1.39	0.93
	Resources (mPt)	2.30	8.98	7.84	4.49	2.10	385.03	9.57	1.45	0.43
LCC	Internal costs ($/kg)	118.2	846.6	578.7	18095.6	761.9	44124.9	1053.8	1230.2	207.6
	External environmental costs ($/kg)	4.69	28.30	16.45	123.25	6.79	498.74	191.88	3.74	2.56
S-LCA	Human resources management	0.203	0.203	0.201	0.1927	0.194	0.1948	0.1927	0.1906	0.198
	Community development	0.240	0.214	0.235	0.2352	0.240	0.1287	0.1768	0.2435	0.248
	Development of society	0.207	0.207	0.207	0.2070	0.207	0.2070	0.2070	0.2070	0.207
	Corporate social Responsibility	0.204	0.204	0.204	0.2048	0.204	0.2048	0.2048	0.2048	0.204

The LCA results show that the microemulsion method has the highest total environmental impacts among the nine nZVI production methods analyzed, significantly higher than the impacts of the other methods. The ultrasonic wave method has the second highest global environmental impacts, followed by reduction with sodium borohydride and reduction with hydrogen gas. The methods with the lowest global environmental impacts are the electrochemical, green synthesis, thermal reduction, and milling methods.

In LCC, the highest life cycle costs were obtained from the microemulsion method, followed by the thermal reduction method. The lowest life cycle costs were obtained from the milling method, followed by the green synthesis method. The costs of the microemulsion method are significantly higher than those of the other methods. In general, in all the methods, the highest costs were the internal costs of the materials. Other costs that also contribute to the life cycle costs of the methods are labor and environmental costs. The labor costs were found to be higher in the methods that require more than 5 h equipment operation, such as in the method of reduction with hydrogen gas and the thermal reduction method. The environmental costs are directly related to the method's environmental impacts, but they did not significantly contribute to the total life cycle costs of the methods.

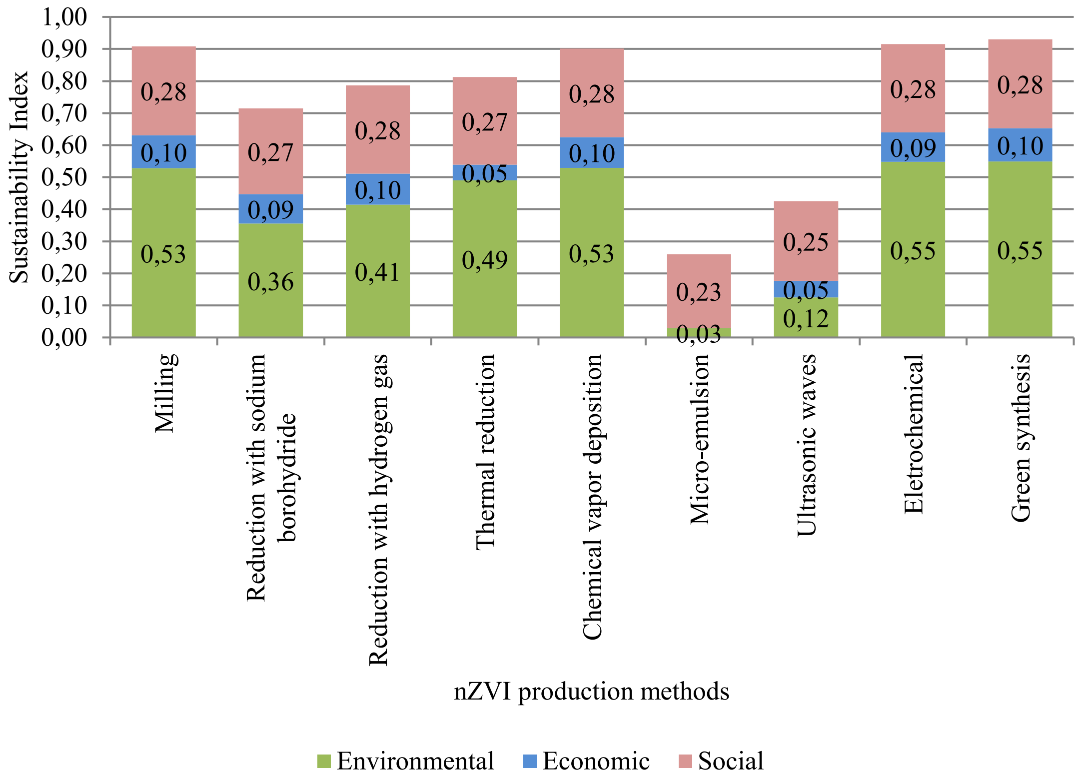
In general, few variations were found in the S-LCA scores of each method (standard deviation: 0.04). However, the milling and green synthesis methods got the highest S-LCA scores (0.856 and 0.853, respectively), and microemulsion (0.735) and the ultrasonic wave method (0.781) got the lowest. The other methods (reduction with hydrogen gas, thermal reduction, chemical vapor deposition, and electrochemical method) got similar scores (around 0.846) and reduction with sodium borohydride got 0.829. Regarding the impact categories, all the methods generally got similar scores.

4.2 Life cycle sustainability assessment

Figure III – 2 shows the sustainability index values of the nine methods of producing 1.00 kg nZVI.

The sustainability index values are expressed on a scale of 0.00–1.00, and the closer the score is to 1.00 the more sustainable the method. The results were expressed through one-dimensional data calculated from the results of the life cycle analyses and normalized with the minimum–maximum function and the weighting factor determined by experts. The sustainability of the methods was classified on the basis of the method of Hossain et al. (2018).

Figure III - 2: Sustainability index values of the nZVI production methods.



The green synthesis method showed the highest sustainability index value, followed by the electrochemical method (with a minimum difference of 0.015), milling, and chemical vapor deposition. These methods were classified as highly sustainable. The differences in sustainability index value among the first four methods are minimal (around 0.03). The thermal reduction method, with the fifth highest sustainability index value (0.83), was also classified as highly sustainable.

The methods of reduction with hydrogen gas and with sodium borohydride have the sixth and seventh highest sustainability index values, and they are classified as sustainable. The methods with the lowest sustainability index values are the ultrasonic wave method and the microemulsion method, classified as neutral and unsustainable, respectively.

The sustainability index values were calculated based on the participation of experts in a multi-criteria analysis using AHP, as described in the methodology section. The weighting factors that were used in this study were the weights found by Visentin et al. (2021a) and shown in Supplementary Material. According to the weighting factors, greater environmental impacts were shown in the impact categories of human health (28.32%) and ecosystem quality (14.32%). Overall, the environmental impact categories were preferred by 57% of the experts; the social categories, by 32%; and the economic impact categories, 10.4% (the lowest). These weighting factor behaviors were verified by the methods' sustainability index values.

- *Green synthesis:* The green synthesis method obtained the highest sustainability index score due to some fundamental factors: its lower environmental impact, low internal and external costs, and high social score. This is a simple and eco-friendly nZVI production method based on the use of plant extracts. This method has numerous advantages in terms of production, such as low cost (green synthesis with plant extract), lower toxicity of the reducing agent used compared to $NaBH_4$, low energy consumption, less toxic waste and effluents generated, increased reactivity of the nZVI particles, and use of natural products (Visentin et al. 2021a). The fact that the production of nZVI through the green synthesis method was shown to be sustainable makes the method ideal for use in laboratories and industry.
- *Electrochemical method:* This method obtained the second highest sustainability index score, with a minimal difference from the score of the green synthesis method. The main factors that contributed to this score were the lower environmental impacts of the method (behind only the green synthesis method), the low external costs, and the high social score. The main advantage of the electrochemical method is that it is a simple method based on electrolysis, which uses simple and available equipment. In addition, the method uses simpler reagents such as iron (III) chloride, but there is a need to use stabilizers and surfactants for the removal of nZVI (Visentin et al. 2021b). Another advantage of the electrochemical method as well as of the green synthesis method is the low energy consumption: 0.04 kWh for the electrochemical method and 0.7 kWh for the green synthesis method. These methods' low energy consumption is directly related to their environmental impacts, which were the lowest among all the analyzed methods. This also explains why such methods have the highest sustainability index environmental scores.
- *Milling:* The main factor contributing to the environmental impacts of the milling method is energy consumption (36 kWh). In the economic aspect the internal costs are related to the iron particle and labor costs (due to the longer equipment operation time for the production of nZVI). The milling method is a simple physical method of producing nZVI requiring only grinding equipment, iron particles, and steel spheres. Another advantage of this method is that it does not use toxic solvents and does not generate residues and effluents. However, nZVI

synthesis occurs after 8 h rotation, resulting in high energy consumption that contributes to the environmental impacts of the method (Visentin et al. 2021a). Because it is a simple, low-cost, and sustainable method, however, it is the favored nZVI production method.

- *Chemical vapor deposition:* The main factor contributing to the sustainability of the method is the use of reagents such as iron pentacarbonate, ethyl, ethylene, and acetylene, and the costs of iron pentacarbonate. This is a simple method of nZVI production, but it is not commonly performed in a laboratory and is not widely used by the scientific community (Crane and Scott 2012; Visentin et al. 2021b). A limiting factor of the method is the cost of iron pentacarbonate, which is about 6.6 times higher than the cost of iron chloride, the main reagent of the green synthesis and electrochemical methods. However, the benefits of the chemical vapor deposition method in the production of nZVI in a non-clustered state, as well as its environmental, economic, social, and sustainability benefits, contribute to the feasibility of its use.
- *Thermal reduction:* This method obtained the fifth highest sustainability index score and was classified as highly sustainable. The main factor that contributes to this method's low sustainability index score is its high production costs. The iron (II) acetate reagent is the most expensive among all the reagents used by the different nZVI production methods analyzed in this study. The high external costs associated with the method's environmental impacts also resulted in a lower sustainability index economic score. However, the method was still classified as highly sustainable because the experts' preference to the internal costs category was the lowest of all categories analyzed. Thus, the environmental and social behaviors of the method favor its sustainability performance. The method's environmental score is one of the highest among the analyzed methods; that is, it has lower environmental impacts. In practical terms, however, the industrial use of this method may be limited due to the high cost of reagents, but in general, the method is sustainable.
- *Reduction with hydrogen gas*: This method's environmental impacts were the main factor that influenced its sustainability index score and its classification as sustainable. This method has been used in the industrial production of nZVI. The main downside of the method is its high energy consumption (112 kWh), which directly influences its environmental impacts. The use of renewable energy, however, favors the industrial use of the method due to the lower environmental

impacts associated with such energy type. The method's costs also make it beneficial to use as these are lower than those of many of the methods analyzed, behind only the milling and green synthesis methods.

- *Reduction with sodium borohydride:* This is the main method used on a laboratory scale for nZVI production (Visentin et al. 2021b). The LCSA in this study demonstrated, however, that this method is one of the three with the lowest sustainability index scores. The main factors associated with the method's low sustainability index score are its environmental impacts and costs, which are directly related to the use of the $NaBH_4$ reagent. According to Visentin et al. (2019), the cost of $NaBH_4$ is associated with its production, for which complex methods are used based on synthetic pathways through the reaction between sodium hydride and trimethylbolate. $NaBH_4$ also contributes to the environmental impacts in the categories of human health and ecosystem quality, which have higher expert preference. However, despite the method's limitations due to its use of $NaBH_4$, the method is classified as sustainable as it is simple and fast and requires readily available equipment.
- *Ultrasonic wave method:* This method obtained the second lowest sustainability index score and is classified as neutral. The main factors associated with this classification are the environmental and economic aspects. The main factor contributing to the environmental impacts of the method are its high energy consumption (62 kWh) and its use of the $NaBH_4$ reagent. In economic terms, the fact that the method has the lowest sustainability index environmental score is due to the method's high external costs, which the experts consider contributing two times more to lower sustainability in the economic aspect than the internal costs. However, the method still has advantages: it is simple and easy to operate, requires readily available equipment, and allows greater control over the morphology of nZVI.
- *Microemulsion:* This method showed the lowest environmental, economic, and social scores in the sustainability index. In this method, high amounts of reagents (above 600 kg in total) are used to produce nZVI. As such, the environmental impacts of nZVI production through this method are higher, and the costs of all the reagents are higher as well. The use of high amounts of reagents in this method is its main disadvantage. As the synthesis of nZVI occurs in the water droplets and oil microemulsions, the production of nZVI is low, thus requiring high amounts of materials (Stefaniuk et al. 2016; Visentin et al. 2021b). In the social

aspects, the use of reagents and the environmental behavior of the method make the method's sustainability index social score the lowest among all the analyzed methods. Thus, the microemulsion method is considered not a sustainable alternative for nZVI production.

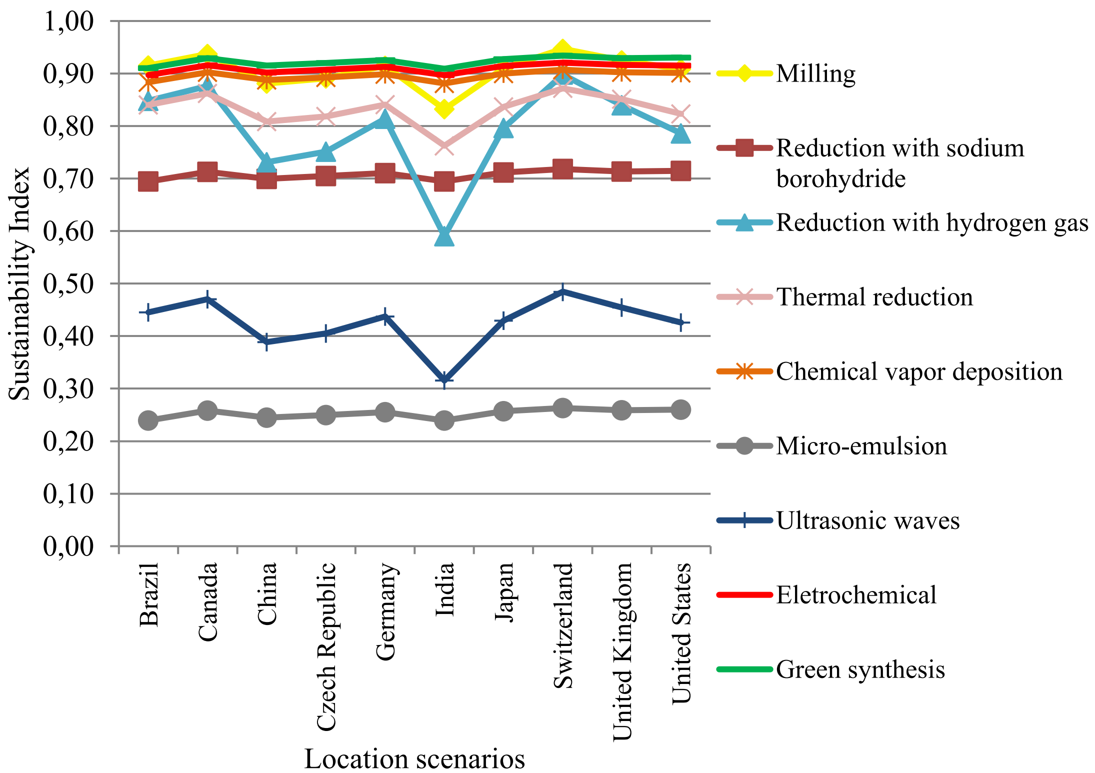
Thus, it was found that the results of the nZVI production methods in the individual life cycle analyses reflect the methods' sustainability index. In addition, the results presented so far were based on the participation of experts in determining the weighting factors of each impact subcategory. Thus, these results reflect the preferences of the group of experts in this study. An analysis considering a different group of experts and different weighting factors will yield different study results. In this sense, sensitivity analysis is important in determining how the changes in the LCSA, such as in the weighting factors, may be reflected in the sustainability index results.

4.3 Complementary analyses

4.3.1 Scenario analysis

Scenario analysis was performed by varying the data location scenario in life cycle analyses results. Figure III - 3 presents the results of the scenario sensitivity analysis.

Figure III - 3: Results of the scenario sensitivity analysis.



In general, it was noticed that the data were not very sensitive to the variation of the data location in the scenarios. The standard deviation of the scenario sensitivity analysis ranged from 0.03 to 0.008. The greatest variations in the sustainability index were noticed in the milling, reduction with hydrogen gas, thermal reduction, and ultrasonic wave methods because these methods have the highest energy consumption (from 36 kWh to 120 kWh). In the other methods, the energy consumption is lower, thus resulting in a smaller variation in the data.

In all the methods, the most sustainable scenario was the Swiss scenario, followed by the Canadian scenario. The Indian scenario was the least sustainable. The behaviors of the methods in these scenarios are mainly based on the methods' environmental impacts, which result in a greater variation than in the economic and social aspects. In Switzerland and Canada, the energy matrix is mainly based on renewable energy, which makes the environmental impacts of the nZVI production methods in these scenarios smaller. On the other hand, in India, the energy matrix is mainly based on non-renewable energies such as coal, making the environmental impacts of the nZVI production methods greater in such scenario.

The economic aspects resulted in minimal variation in the scenarios considered due to the low costs of industrial energy, and in many cases, the energy consumption is also low. The external costs were the ones that varied the most in the economic aspects due to the behaviors of the methods in the environmental analysis, but the variation in these scenarios did not result in a larger contribution in the sustainability behaviors of the methods. The Indian scenario showed the highest life cycle costs of the methods while the Canadian and Swiss scenarios showed the lowest ones.

The social aspects varied in all the scenarios considered, but this variation was also minimal (about 10%). The lowest social scores were found in the Indian and Brazilian scenarios. In these scenarios, the social indicators have lower scores, thus reflecting the social realities in these countries. On the other hand, the Swiss scenario resulted in the highest social scores.

Another factor that can be highlighted is that there are changes in the sustainability classifications of the reduction with hydrogen gas, thermal reduction, and ultrasonic wave methods in the Indian scenario. In this scenario, the thermal reduction method goes from highly sustainable to sustainable while the method of reduction with hydrogen gas goes from sustainable to neutral. In the ultrasonic wave method, the classification goes from neutral to unsustainable in the Indian and Chinese scenarios.

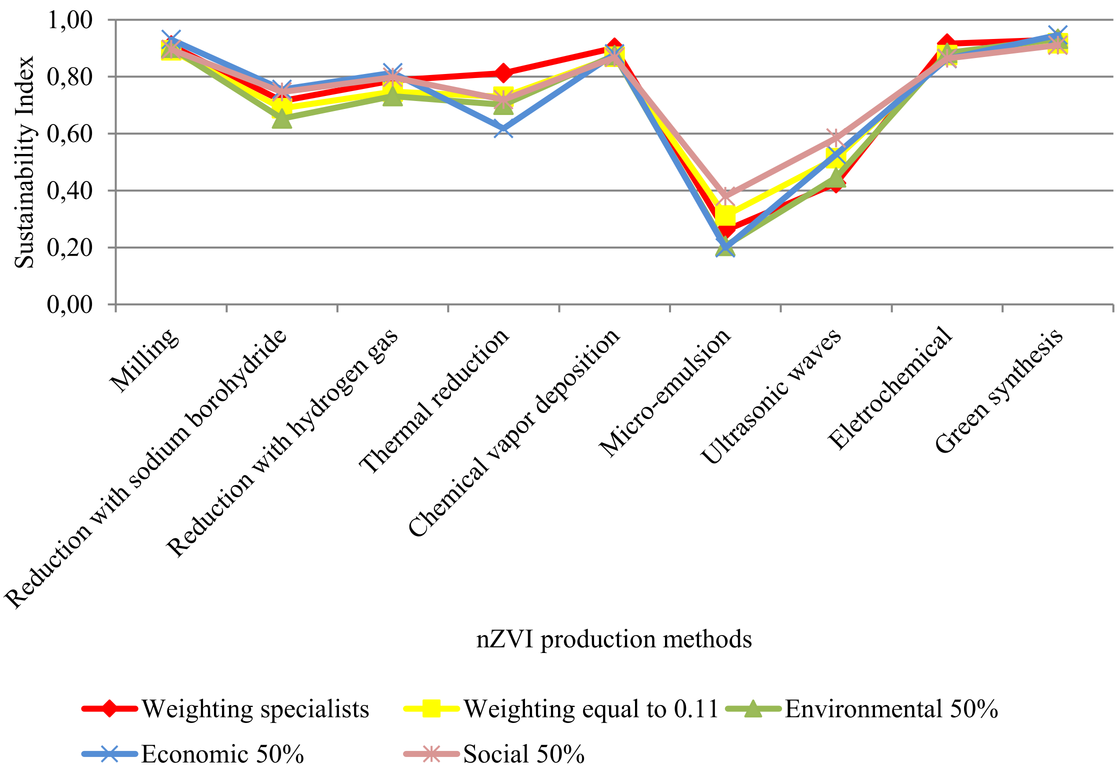
In the Swiss and Canadian scenarios, for example, the method with the highest sustainability index value is the milling method, surpassing the sustainability index value of the green synthesis method. Thus, locating inventory data on the sustainability behaviors of the methods is perceived as important. The sustainability index will reflect the environmental, economic, and social behaviors of the localization scenario.

4.3.1.1 Weighting factor analysis

The sensitivity analysis of the weighting factors was performed in three variations: (1) weighting factor equal to 0.11 for all the impact categories; (2) the experts' preference for the environmental, economic, and social aspects; and (3) ± 20% variation in the weighting factors chosen by the experts.

Figure III - 4 presents the results of the first and second variation considering, the weighting factors equal to 0.11 for all the impact categories and the preference sensitivity of the three different aspects, comparing these with the results of the analyses when equal weighting factors were given for all the impact categories.

Figure III - 4: Results of the sensitivity analysis considering the weighting factor equal to 0.11 for all the impact categories and the preference sensitivity analysis of the sustainability aspects.



The analysis of the weighting factor equal to 0.11 for all the impact categories demonstrated that the results are not very sensitive to this type of variation. Overall, the use of equal weighting factors for all the impact categories resulted in a lower sustainability index value than when the experts' opinions were considered. This is because in the experts' analysis, some impact categories are more important than the others. On the other hand, in the microemulsion and ultrasonic wave methods, the use of equal weighting factors increased the sustainability index value. Moreover, the classification of the sustainability of the methods was not modified in the variation considered. Thus, it is perceived that LCSA can be performed with or without considering the opinions of experts in defining the weighting factors.

The use of experts promotes a more significant analysis because it considers the preference of each expert in relation to the impact categories, and in practice and considering different contexts; the preferences are not always the same. On the other hand, sustainability in essence considers the environmental, economic, and social aspects on an equal; thus, the use of equal weighting factors results in a more transparent and egalitarian analysis. As for LCSA, there is no method indicated for it; it is up to each author, in his or her context, to consider or not to consider experts' opinions or whether to give equal weighting factors or not to.

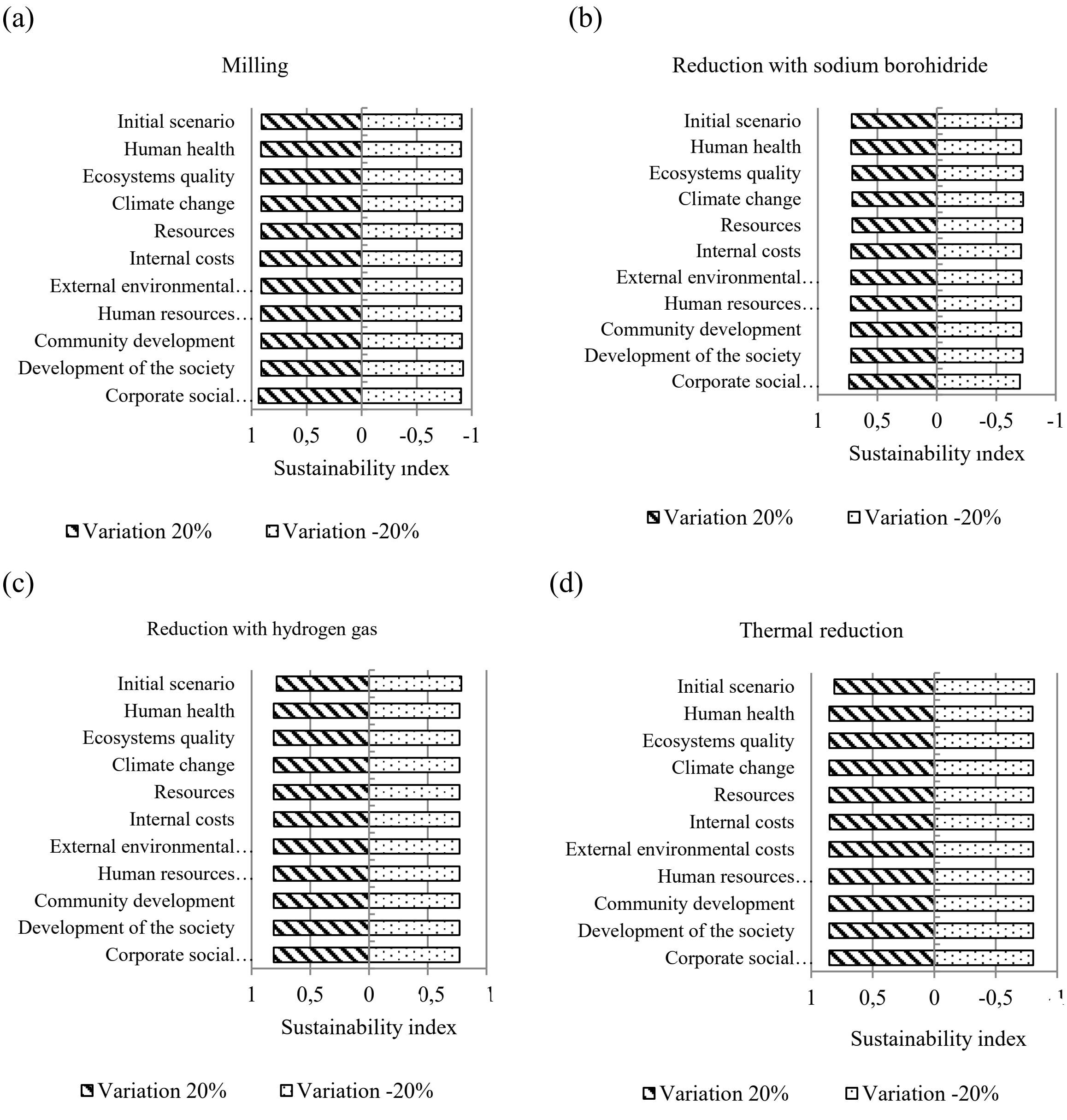
It is noteworthy that in this work weighting factors were used for the impact categories of the endpoint of each sustainability aspect and not for the aspects themselves. This type of analysis has been shown to be more accurate because it compares all the impact categories of the life cycle analyses to each other, which results in more precise preferences than if only the environmental, economic, and social aspects are compared.

The second sensitivity analysis of the sustainability index results on the basis of weighting factors given was performed considering the superior preference of experts for each sustainability aspect (Figure 4). Thus, three analyses were carried out: (1) that with a 50% preference or weighting factor given by experts to the environmental aspect (economic aspect, 25%; social aspect, 25%); (2) that with a 50% preference or weighting factor given by experts to the economic aspect (environmental aspect, 25%; social aspect, 25%); and (3) that with a 50% preference or weighting factor given by experts to the social aspect (environmental aspect, 25%; economic aspect, 25%).

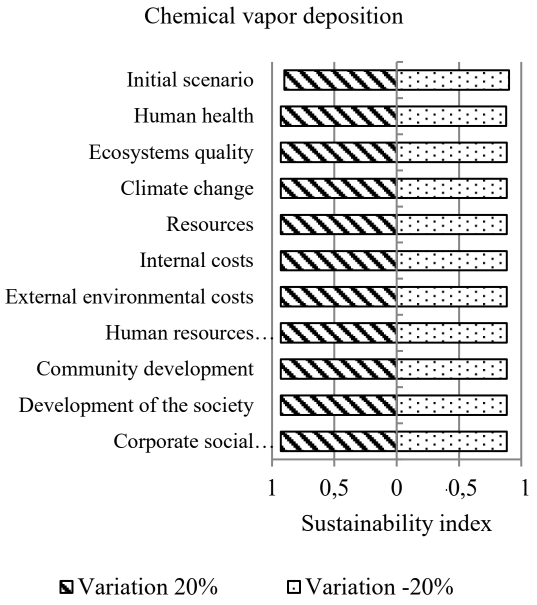
Considering the preferences among the environmental, economic, and social aspects, it is perceived that the results are not very sensitive to this analysis. Overall, the standard deviation of the sustainability index results of the methods in this sensitivity analysis ranged from 0.013 (chemical vapor deposition) to 0.07 (microemulsion method).

The last variation scenario evaluated in the weighting factor sensitivity analysis involved a ± 20% variation in the weights given by the experts to the impact categories. The weights of the other categories were adjusted by ± 2.5% so that their sum would be equal to 1.00. Figure III - 5 (a) to 5 (i) presents the results of this analysis of each nZVI production method.

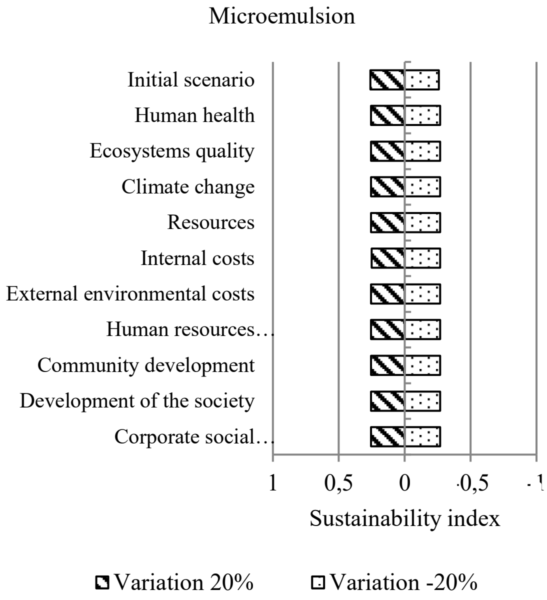
Figure III - 5: Sensitivity analysis with a ± 20% variation of the weighting score.



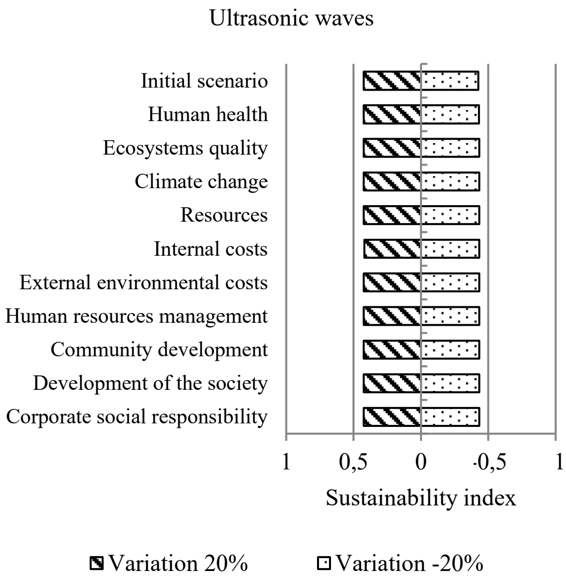
(e)


Chemical vapor deposition
Initial scenario
Human health
Ecosystems quality
Climate change
Resources
Internal costs
External environmental costs
Human resources…
Community development
Development of the society
Corporate social…
1
0,5
0
0,5
1
Sustainability index
Variation 20%
Variation -20%

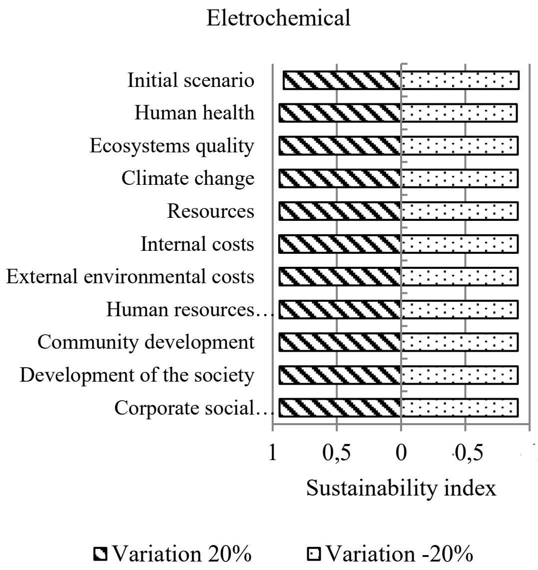
(f)


Microemulsion
Initial scenario
Human health
Ecosystems quality
Climate change
Resources
Internal costs
External environmental costs
Human resources…
Community development
Development of the society
Corporate social…
1
0,5
0
0,5
Sustainability index
Variation 20%
Variation -20%

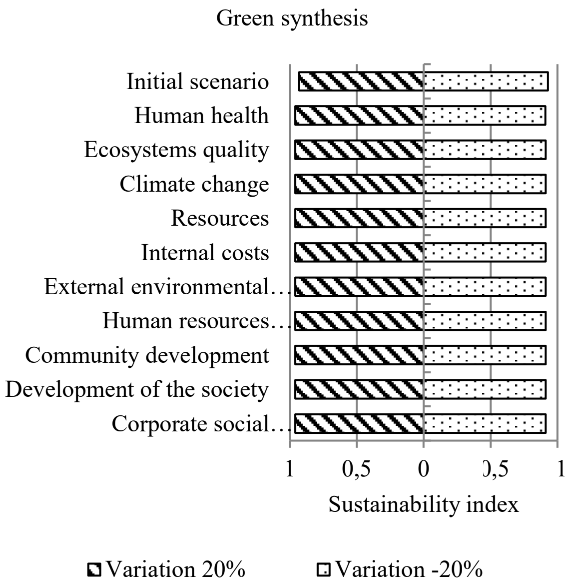
(g)


Ultrasonic waves
Initial scenario
Human health
Ecosystems quality
Climate change
Resources
Internal costs
External environmental costs
Human resources management
Community development
Development of the society
Corporate social responsibility
1
0,5
0
0,5
1
Sustainability index
Variation 20%
Variation -20%

(h)


Eletrochemical
Initial scenario
Human health
Ecosystems quality
Climate change
Resources
Internal costs
External environmental costs
Human resources…
Community development
Development of the society
Corporate social…
1
0,5
0
0,5
Sustainability index
Variation 20%
Variation -20%

(i)

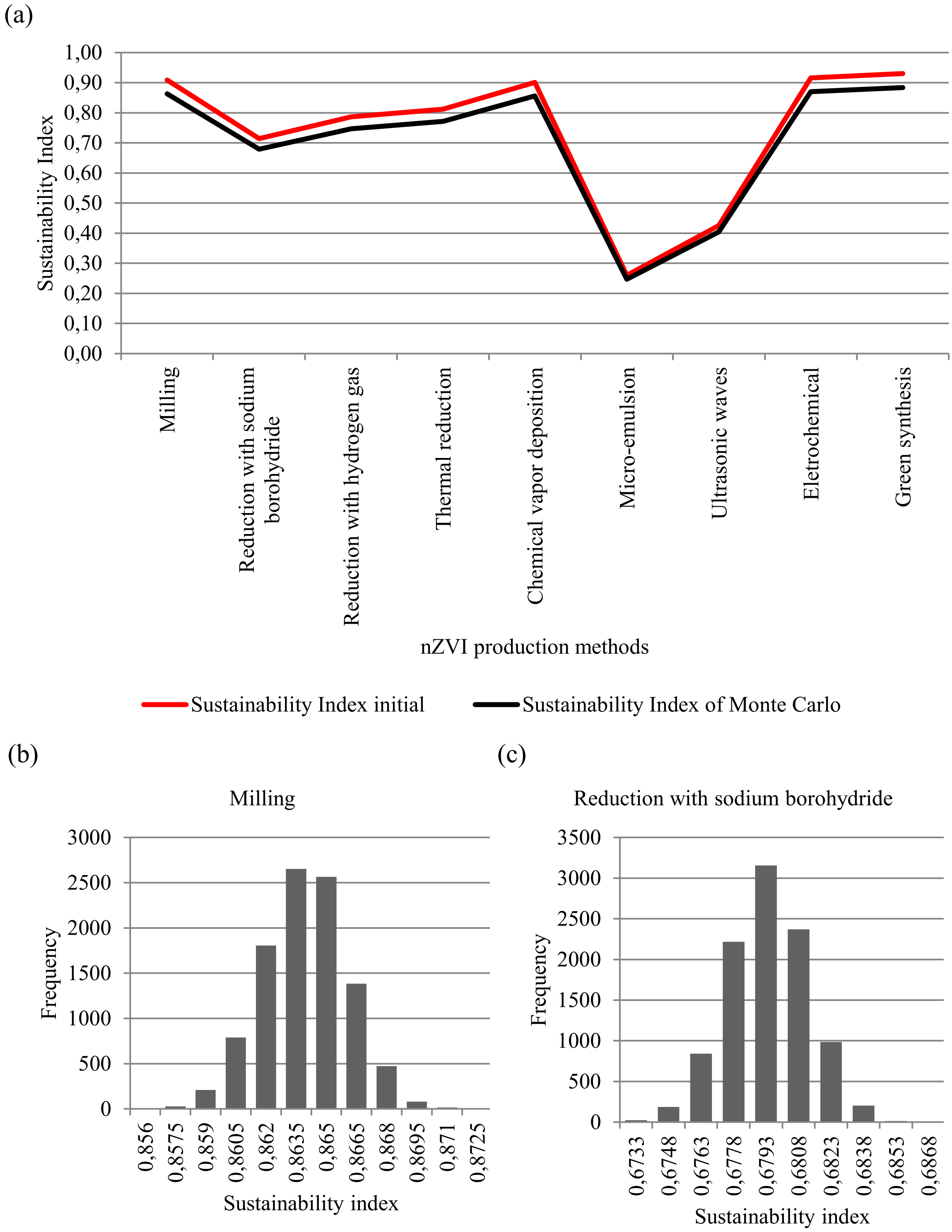


The results of the sensitivity analysis involving a ± 20% variation in the weights given by the experts to the impact categories are not very sensitive to the changes in the weights of such impact categories, with minimal variance. In addition, the methods' sustainability classifications were not altered in this analysis.

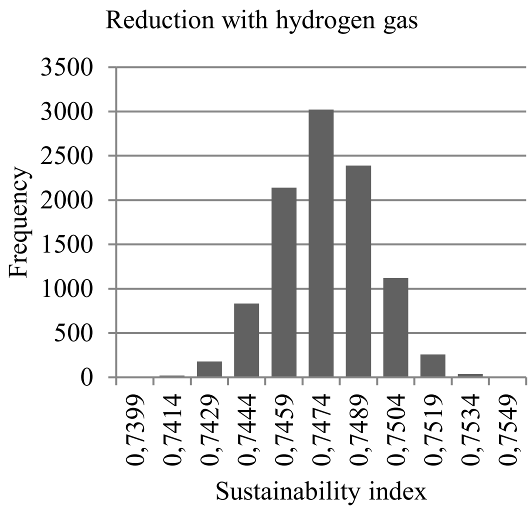
4.1.1.2 Uncertainty analysis

Figure III – 6 shows the results of the Monte Carlo simulation of the sustainability index value of each nZVI production method. In the Supplementary Material are presented the Monte Carlo histograms of each method.

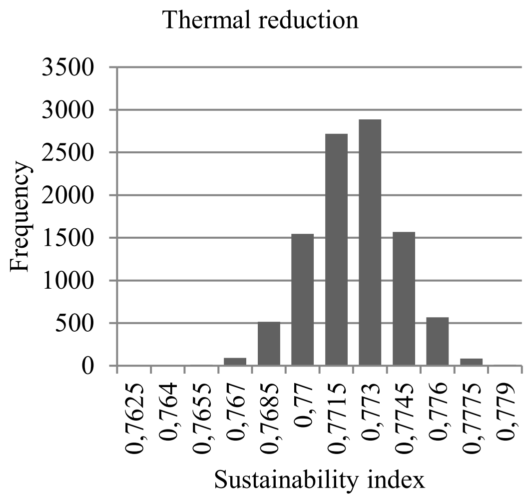
Figure III - 6: Results of the Monte Carlo simulation of the sustainability index values of the nZVI production methods.



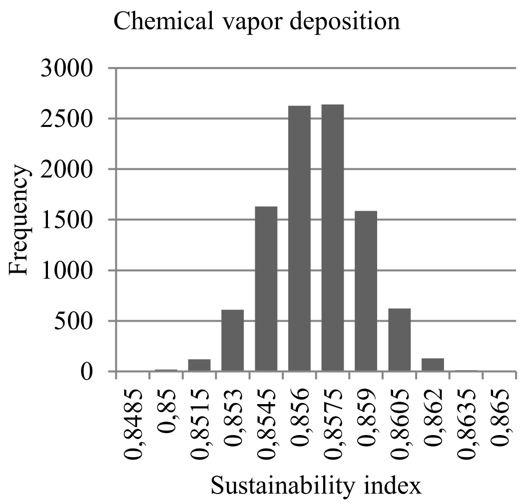
(d)


Reduction with hydrogen gas
3500
3000
2500
2000
1500
1000
500
0
Frequency
0,7399
0,7414
0,7429
0,7444
0,7459
0,7474
0,7489
0,7504
0,7519
0,7534
0,7549
Sustainability index

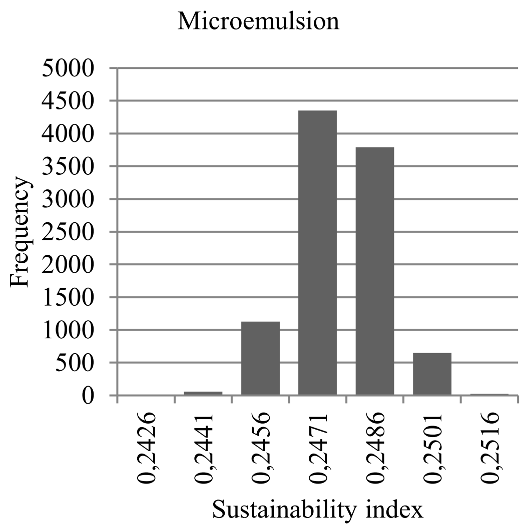
(e)


Thermal reduction
3500
3000
2500
2000
1500
1000
500
0
Frequency
0,7625
0,764
0,7655
0,767
0,7685
0,77
0,7715
0,773
0,7745
0,776
0,7775
0,779
Sustainability index

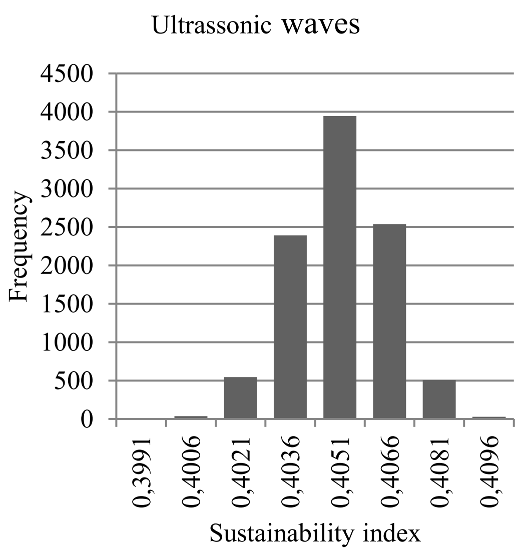
(f)


Chemical vapor deposition
3000
2500
2000
1500
1000
500
0
Frequency
0,8485
0,85
0,8515
0,853
0,8545
0,856
0,8575
0,859
0,8605
0,862
0,8635
0,865
Sustainability index

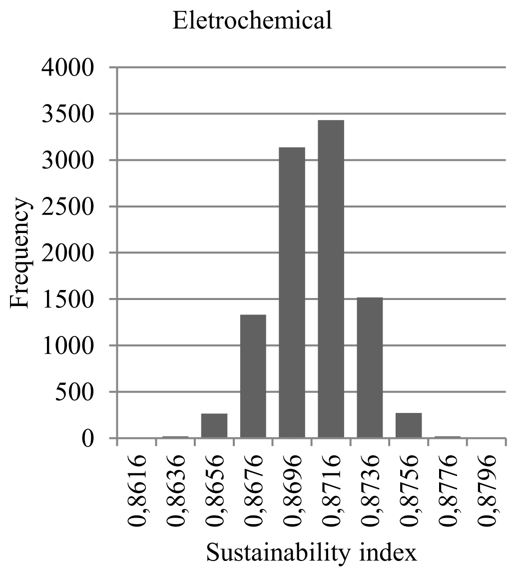
(g)


Microemulsion
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
Frequency
0,2426
0,2441
0,2456
0,2471
0,2486
0,2501
0,2516
Sustainability index

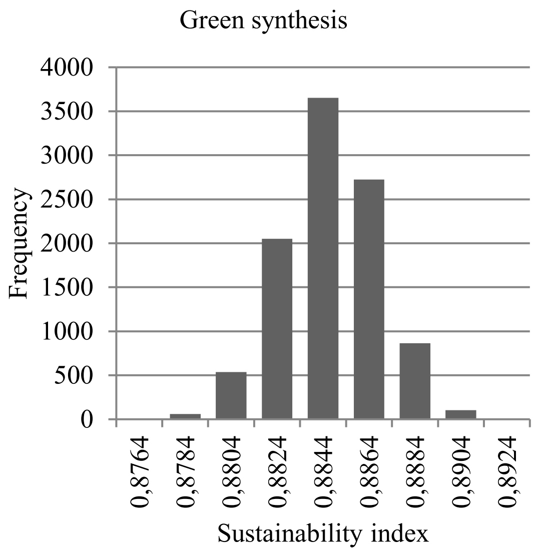
(h)


Ultrassonic waves
4500
4000
3500
3000
2500
2000
1500
1000
500
0
Frequency
0,3991
0,4006
0,4021
0,4036
0,4051
0,4066
0,4081
0,4096
Sustainability index

(i)


Eletrochemical
4000
3500
3000
2500
2000
1500
1000
500
0
Frequency
0,8616
0,8636
0,8656
0,8676
0,8696
0,8716
0,8736
0,8756
0,8776
0,8796
Sustainability index

(j)



The sustainability index values determined via Monte Carlo simulation are more accurate than those determined by the traditional method used in this research, but it was noticed that there was little variation between the index values, resulting in a low standard deviation (minimum: 0.009; maximum: 0.032). In addition, the sustainability classifications of the methods did not change the results of the Monte Carlo simulation. Thus, it is important to consider the analysis of uncertainties in LCSA to improve its implementation and to reduce its uncertainties.

5. Conclusion

LCA, LCC, S-LCA, and LCSA were applied to nine nZVI production methods. The green synthesis method is the most sustainable nZVI production method while the microemulsion method is the least sustainable. The green synthesis, electrochemical, milling, chemical vapor deposition, and thermal reduction methods are classified as highly sustainable. The methods of reduction with hydrogen gas and with sodium borohydride are classified as sustainable. The ultrasonic wave method is classified as neutral, and the microemulsion method, as unsustainable.

The scenarios analysis showed that in general, the results are not very sensitive to variation, with a low standard deviation. However, the Swiss and Canadian scenarios resulted in the highest sustainability index values for all the methods while the Indian scenario resulted in the lowest. The sensitivity analysis of the weighting factors also demonstrated that the results are not very sensitive to variations in weighting factors.

Finally, this study addressed a specific research gap by providing a detailed LCSA of nine nZVI production methods. The study is essential because nanomaterials are becoming increasingly present in people's daily lives (e.g., pharmaceuticals, electronics, and food) and in environmental remediation processes. Therefore, understanding the sustainability of the methods of producing nZVI, which is applied to the remediation of contaminated sites, can help decision makers choose the best remediation alternatives to use in a given location considering all the environmental, social, and economic aspects of such alternatives.

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Author Contribution Statements

Visentin, C. and Braun, A. B. contributed to the study conception and design. Material preparation, data collection, and analysis were performed by Visentin, C.; Braun, A. B., Trentin, A. W. da Silva. The first draft of the manuscript was written by Visentin, C. and Braun, A. B. Thomé, A. was responsible for the revision of the manuscript. All authors commented on previous versions of the manuscript and the revision. All authors read and approved the final manuscript.

Author Disclosure Statement

No competing financial interests exist.

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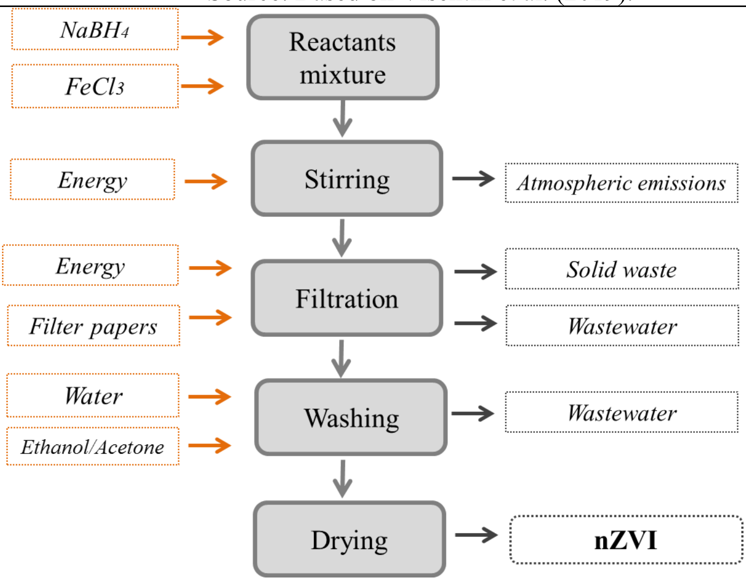
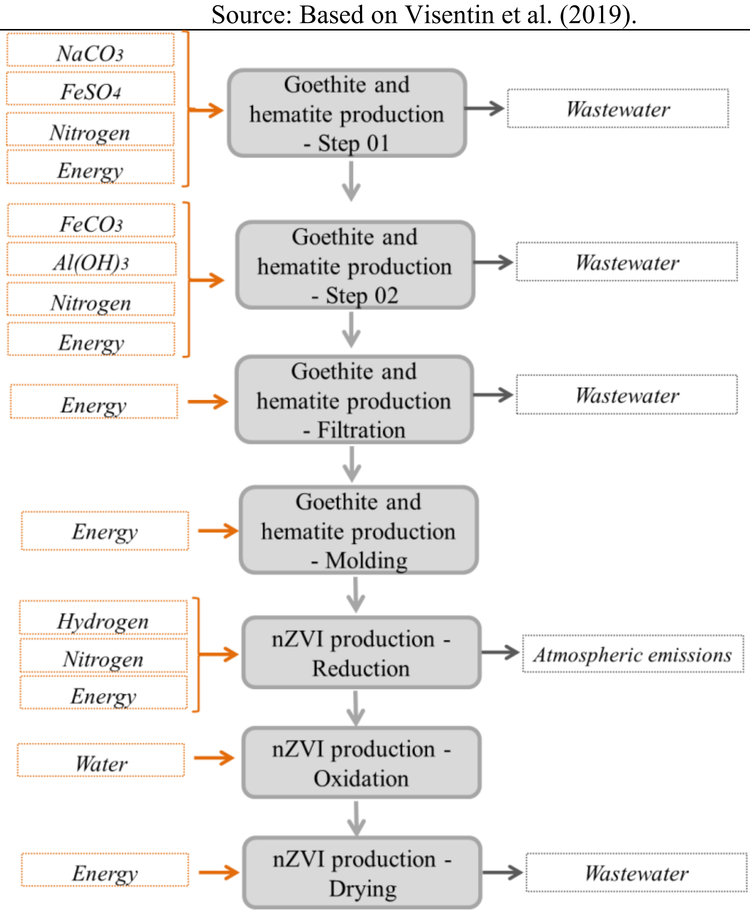
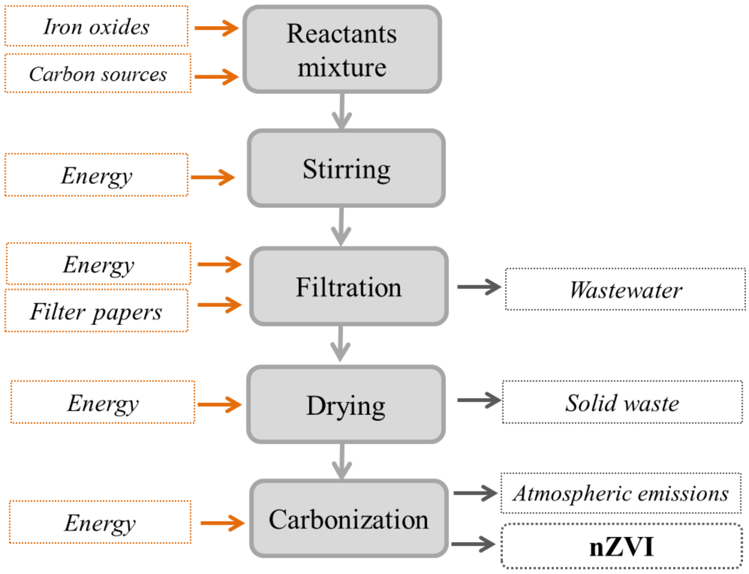
Supplementary Material

Table III - 3: Production flowchart of nZVI production methods

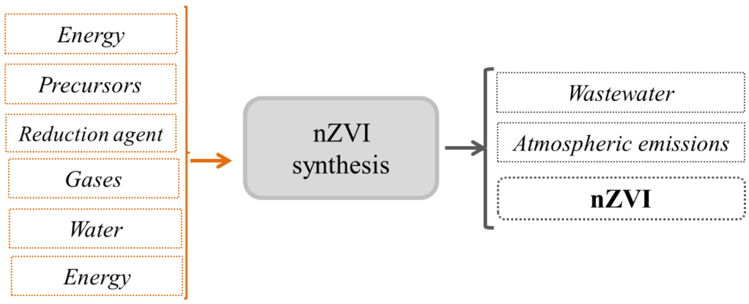
Methods	Production flowchart
Milling	 Source: Based on Visentin et al. (2019).
Chemical reduction with sodium borohydride	 Source: Based on Visentin et al. (2019).
Chemical reduction with hydrogen gas	 Source: Based on Visentin et al. (2019).

Methods	Production flowchart

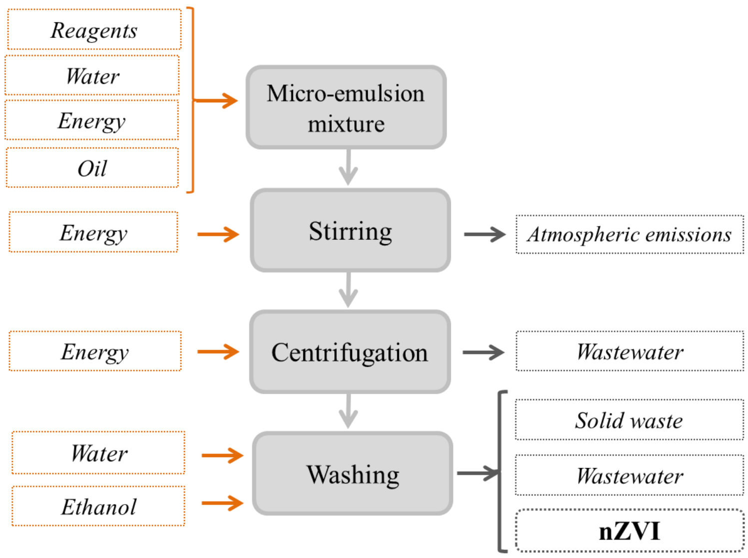
Thermal reduction



Chemical vapor deposition

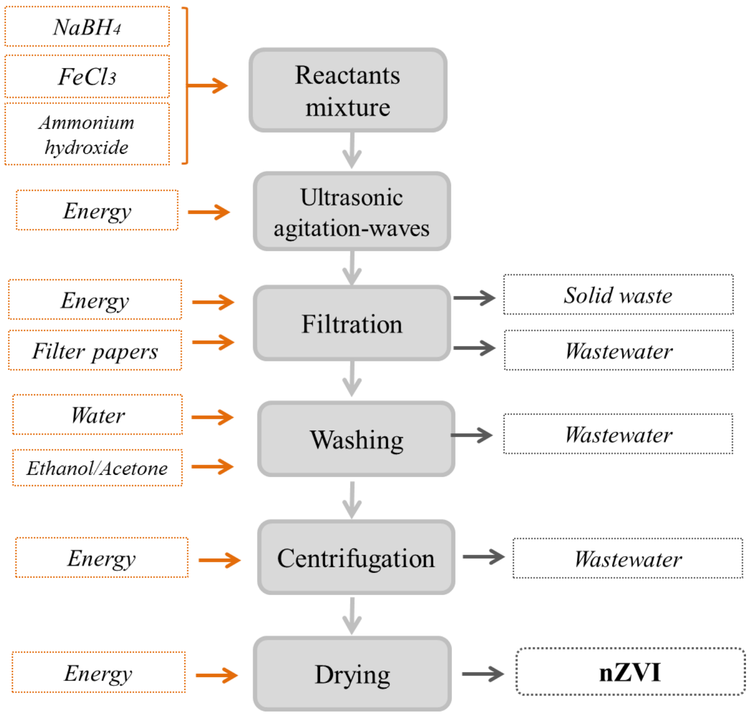


Micro emulsion

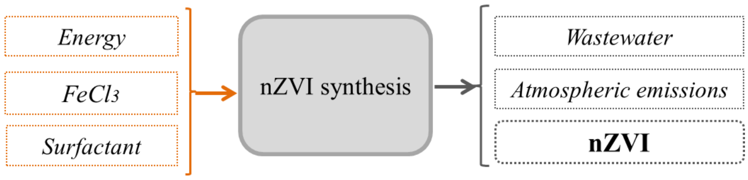


Methods — **Production flowchart**

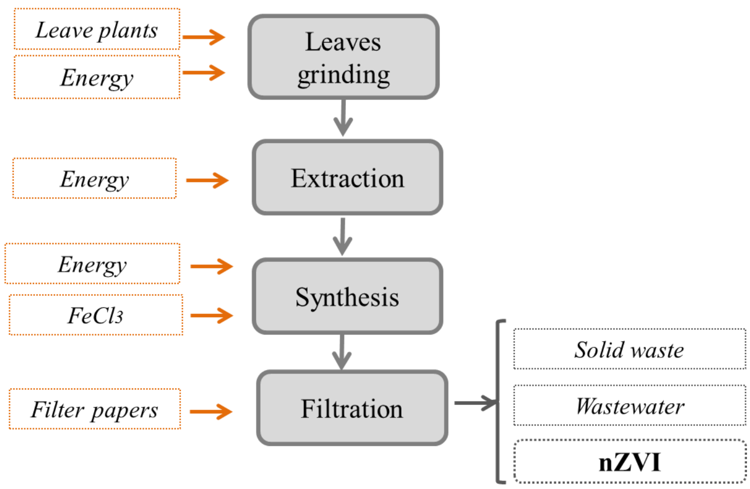
Ultrasonic waves



Eletrochemical



Green synthesis



Source: Based on Martins et al. (2017).

Inventory and operational detailing of methods

Table III - 4: Environmental and economic inventory data of the nZVI production methods.

Method	Production stages	Inputs and outputs	Amount	Costs
Milling	Milling	Iron particles	1.00 kg	87.5 $/kg
		Energy	36 kWh	0.06 $/kWh
		Stell ball	1.8 kg	
		Atmospheric emissions	2.00×10^{-4} g	
		Labor costs	8 h	7.25 $/h
Liquid chemical reduction with Sodium borohydride	Mixing of reagents	Iron chloride (III) - $FeCl_3$	2.9 kg	41.60 $/kg
		Sodium borohydride - $NaBH_4$	2.71 kg	303.00 $/kg
	Stirring	Energy	7.5×10^{-2} kWh	0.06 $/kWh
	Filtration	Energy	1.05×10^{-1} kWh	0.06 $/kWh
		Paper filters	2.49 kg	32.75 $/kg
		Solid waste	2.49 kg	1.20 $/kg
		Wastewater	7.16×10^{-2} m³	0.15 $/m³
	Washing	Ethanol	4.76×10^{-3} m³	0.07 $/m³
		Deionized water	1.96×10^{-1} m³	0.04 $/m³
		Wastewater	2.13×10^{-1} m³	0.15 $/m³
		Labor costs	1 h	7.25 $/h
Gaseous chemical reduction with hydrogen gas	Goethite and hematite production - step 01	Sodium carbonate - $NaCO_3$	3.55 kg	39.98 $/kg
		Iron sulfate (II) - $FeSO_4$	2.49 kg	166.00 $/kg
		Nitrogen - N_2 (gas)	5.87×10^{-1} kg	0.04 $/kg
		Energy	6.72 kWh	0.06 $/kWh
		Wastewater	2.07×10^{-3} m³	0.15 $/m³
	Goethite and hematite production - step 02	Iron carbonate - $FeCO_3$	2.62 kg	9.98 $/kg
		Aluminium hydroxide – $Al(OH_3)$	8.42×10^{-2} kg	90.50 $/kg
		Nitrogen - N_2 (gas)	2.07 kg	0.04 $/kg
		Energy	33.6 kWh	0.06 $/kWh
		Wastewater	11.03×10^{-3} m³	0.15 $/m³
	Goethite and hematite production - Filtration	Energy	4×10^{-2} kWh	0.06 $/kWh
		Wastewater	9.27×10^{-3} m³	0.15 $/m³
	Goethite and Hematite Production - Molding	Energy	15.2 kWh	0.06 $/kWh
	nZVI production - Reduction	Energy	55.2 kWh	0.06 $/kWh
		Hidrogen - H_2 (gas)	5.8×10^{-2} kg	0.04 $/kg
		Nitrogen - N_2 (gas)	3.22×10^{-3} kg	0.04 $/kg
		Water (vapor)	5.19×10^{-1} kg	
	nZVI production - Oxidation	Deionized water	5.00×10^{-3} m³	0.04 $/m³
	nZVI production - Drying	Energy	4.8×10^{-1} kWh	0.06 $/kWh
		Wastewater	4.00×10^{-3} m³	0.15 $/m³
		Labor costs	18 h	7.25 $/h

Method	Production stages	Inputs and outputs	Amount	Costs
Thermal reduction	Mixing of reagents	Iron nitrate – Fe $(NO_3)_3.9H_2O$	2.832 kg	140.80 $/kg
		Carbon black	0.283 kg	0.70 $/kg
		Deionized water	$1.15x10^{-2}$ m³	0.004 $/m³
	Stirring	Energy	$7.50x10^{-2}$ kWh	0.06 $/kWh
	Filtration	Energy	$2.07x10^{-2}$ kWh	0.06 $/kWh
		Nylon membrane	0.5 kg	53.00 $/kg
		Wastewater	$1.15x10^{-2}$ m³	0.15 $/m³
		Solid waste	0.5 kg	1.20 $/kg
	Drying	Energy	28.8 kWh	0.06 $/kWh
		Solid waste	1.11 kg	1.20 $/kg
	Carbonization	Iron acetate (II) - $Fe(C_2H_3O_2)_2$	3.117 kg	7080.00 $/kg
		Argon	7.96 $x10^{-2}$ kg	0.02 $/kg
		Energy	4.8 kWh	0.06 $/kWh
		Atmospheric emissions (Argon, CH_2CO, CO, H_2O)	$5.56x10^{-1}$ m³	
	Labor costs		17 h	7.25 $/h
Chemical vapor dopsosition	Synthesis	Iron pentacarbonate - $Fe(CO)_5$	2.8 kg	276.00 $/kg
		Ethyl - C_2H_5	$3.6x10^{-2}$ kg	14.67 $/kg
		Ethylene - C_2H_4	$1.6x10^{-2}$ kg	3481.00 $/kg
		Acetylene - C_2H_2	$5.4x10^{-2}$ kg	0.09 $/kg
		Argon	8.0 kg	0.02 $/kg
		Atmospheric emissions (particulate matter, argon)	9.66 kg	
		Energy	1.2 kWh	0.06 $/kWh
	Labor costs		2 h	7.25 $/h
Micro-emulsion	Preparation and mixing of micro-emulsions	Iron sulfate (II) - $FeSO_4$	2.7 kg	166.00 $/kg
		Potassium tetrahydroborate - KBH_4	$9.6x10^{-1}$ kg	524.00 $/kg
		Surfactant	177.74 kg	214.00 $/kg
		n-butanol	88.87 kg	16.20 $/kg
		Isooctano	355.5 kg	41.40 $/kg
		Deionized water	$10.3x10^{-2}$ m³	0.04 $/m³
		Energy	$7.50x10^{-2}$ kWh	0.06 $/kWh
	Nanoparticles separation	Argon	$3.3x10^{-3}$ kg	0.02 $/kg
		Wastewater	$6.4x10^{-1}$ m³	0.15 $/m³
	Washing	Deionized water	$1.0x10^{-2}$ m³	0.04 $/m³
		Anhydrous ethanol	3.0x 10^{-2} m³	0.07 $/m³
		Acetone	$3.0x10^{-2}$ m³	0.03 $/m³
		Argon	$9.9x10^{-3}$ kg	0.02 $/kg
		Wastewater	$1.4x10^{-1}$ m³	0.15 $/m³
	Drying	Argon	$3.3x10^{-3}$ kg	0.02 $/kg
		Energy	1.2 kWh	0.06 $/kWh
		Atmospheric emissions	$8.9x10^{-2}$ m³	
	Labor costs		2 h	7.25 $/h

Method	Production stages	Inputs and outputs	Amount	Costs
Ultrasonic wave	Preparation of reagents	Iron sulfate (II) - $FeSO_4.7H_2O$	4.978 kg	166.00 $/kg
		Sodium borohydride - $NaBH_4$	1.35 kg	303.00 $/kg
		Ethanol	$2.22x10^{-1}$ m³	0.07 $/kg
		Deionized water	$9.03x10^{-2}$ m³	0.04 $/m³
		Energy	$1.25x10^{-2}$ kWh	0.06 $/kWh
	Agitation with ultrasonic waves	Energy	3.90 kWh	0.06 $/kWh
		Nitrogen	$5.82x10^{-1}$ kg	0.04 $/kg
		Deionized water	$2.00x10^{-2}$ m³	0.04 $/m³
		Atmospheric emissions	$2.52x10^{-1}$ kg	
	Filtration	Energy	$2.5x10^{-2}$ kWh	0.06 $/kWh
		Nylon membrane	0.5 kg	53.00 $/kg
		Solid waste	0.65 kg	1.20 $/kg
		Wastewater	$1.32x10^{-1}$ m³	0.15 $/m³
	Washing	Ethanol	$6.19x10^{-2}$ m³	0.07 $/m³
		Wastewater	$6.19x10^{-2}$ m³	0.15 $/m³
	Centrifugation	Energy	$5.8x10^{-2}$ kWh	0.06 $/kWh
		Wastewater	$2.48x10^{-2}$ m³	0.15 $/m³
	Drying	Energy	57.6 kWh	0.06 $/kWh
	Labor costs		3 h	7.25 $/h
Electrochemical	Preparation of reagents	Iron chloride (III) - $FeCl_3$	1.16 kg	41.60 $/kg
		Deionized water	$7.20x10^{-3}$ m³	0.04 $/m³
		Energy	$1.25x10^{-2}$ kWh	0.06 $/kWh
	nZVI production	Deionized water	$1.00x10^{-2}$ m³	0.04 $/m³
		Polyvinylpyrrolide (PVP)	$7.2x10^{-1}$ kg	252.00 $/kg
		Cetylpiridium chloride (CPC)	1.4 kg	924.00 $/kg
		Energy	$2x10^{-1}$ kWh	0.06 $/kWh
		Wastewater	$1.72x10^{-2}$ m³	0.15 $/m³
		Atmospheric emissions	$7.6x10^{-1}$ kg	
	nZVI collection	Argon	$9.9x10^{-3}$ kg	0.02 $/kg
		Deionized water	$2.0x10^{-3}$ m³	0.04 4/m³
		Wastewater	$1.00x10^{-2}$ m³	0.15 $/m³
	Labos costs		2 h	7.25 $/h
Green synthesis	Grinding of leaves	Leaves	1.8 kg	21.90 $/kg
		Energy	$3.5x10^{-1}$ kWh	0.06 $/kWh
	Extraction	Deionized water	$5.00x10^{-2}$ m³	0.04 $/m³
		Energy	$3.3x10^{-1}$ kWh	0.06 $/kWh
	Syntheis	Iron chloride (III) - $FeCl_3$	2.90 kg de	41.60 $/kg
		Energy	$4x10^{-2}$ kWh	0.06 $/kWh
	Filtration	Energy	$4.2x10^{-2}$kWh	0.06 $/kWh
		Paper filters	2.49 kg	32.75 $/kg
		Solid waste	2.83 kg	1.20 $/kg
		Wastewater	$4.9x10^{-2}$ m³	0.15 $/m³
	Labor costs		2 h	7.25 $/h

External environmental costs	Global warming	kg CO_2 eq	$0.14
	Eutrophication	kg PO_4 P-lim	$4.56
	Acidification	kg SO_2 eq	$9.60
	Depletion of the ozone layer	kg CFC-11 eq	$387.86
	Photochemical oxidation	kg C_2 H_4 eq	$2.47
	Inorganic respirators	kg PM2.5 eq	$39.78

The inventory data of the milling, reduction with sodium borohydride, and reduction with hydrogen gas methods were obtained from Visentin et al. (2019b); those of the thermal reduction method, from Hoch et al. (2008); those of chemical vapor deposition, from Dumitrache et al. (2004); those of microemulsion, from Zhang et al. (2007); those of the ultrasonic wave method, from Jamei et al. (2014); those of the electrochemical method, from Chen et al. (2004); and those of green synthesis, from Martins et al. (2017).

For the grinding method, the 8-hour operation of the planetary ball mill with a power of 11.25 kW was considered. For the sodium borohydride reduction method the equipment used is magnetic agitator with a power of 150 W, with operation for 30 minutes, and vacuum filter with a power of 125 W and operation of 5 minutes. In the hydrogen gas reduction method the considerations were: (i) in the production stages of goethite reduction equipment with power of 16.8 kW, operating for 70 minutes in the first step, and 5 h in the second; filter press with a power of 100 W operating for 2 h; and 38 kW molding and compression machine operating for 1 h. (ii) in the production stages of nZVI, the reduction equipment with a power of 46 kW and operation of 180 minutes, and drying kiln with power of 200 W operating for 6 h.

The inventory data for the thermal reduction method were obtained by means of estimates according to the work of Hoch et al. (2008) which applied the method in the production of nZVI. In addition, some considerations were made: (i) operation of the 30-minute stirring equipment with a power of 150 W; (ii) operation of the vacuum filtration equipment for 10 minutes (equipment power of 125 W); (iii) drying oven with power of 6 kW operating for 12 h; (iv) pipe oven with power of 3 kW operating for 4 h. The nylon membrane used in the method was 47 mm in diameter according to Hoch et al. (2008).

In the vapor deposition method, the data were obtained by means of estimates according to the work of Dumitrache et al. (2004). Some considerations were made: (i) the laser power of 100 W, operating for 10 minutes; (ii) continuous flow reactor with 3kWh power operating for one hour.

The inventory data for the micro-emulsion method were obtained by means of estimates according to the work of Zhang et al. (2007). Some considerations were made: (i) the power of the agitator in the preparation and mixing stage of the micro-emulsions is 150W operating for 30 minutes; (ii) in the drying step a 3kW kiln operating for one hour.

In the ultrasonic wave method, inventory data were obtained by means of estimates according to the work of Jamei et al. (2014) which applied the method in the production of nZVI. In addition, some considerations were made: (i) operation of the 5-minute stirring equipment with a power of 150 W; (ii) ultrasonic wave stirring stage equipment was a Hielscher Company's sonification device (UIP 1000 hd) with 1kW power operating for 30 minutes; generator with power of 17 kW operating for 30 minutes; and a heating with a power of 1.5 kW operating for 30 minutes; (iii)operation of the vacuum filtration equipment for 20 minutes (equipment power of 125 W); (iv) centrifuge with power of 350 W operating for 10 minutes (v) pipe oven with power of 3 kW operating for 24 h.

The inventory data for the electrochemical method were obtained by means of estimates according to the work of Chen et al. (2004) which applied the method in the production of nZVI. In addition, some considerations were made: (i) operation of the 5-minute stirring equipment with a power of 150 W; (ii) the power supply of the nZVI production step with 300 W power operating for 30 minutes, and the ultrasonic vibrator (Enshine UC-300.20 kHz) with 1kW power operating for 30 minutes.

In the green synthesis method, inventory data were obtained through estimates according to Martins' work. (2017) that applied the method in the production of nZVI. In addition, some considerations were made: (i) operation of the equipment to grind the 30-minute foliage with a power of 700 W; (ii) in the extraction step a magnetic stirrer with heating with power of 1 kW operating for 30 minutes; (iii) in the synthesis stage stirring equipment with power of 150 W operating for 20 minutes; (iv) filtration equipment with power of 125 W operating for 20 minutes.

Table III - 5: Impact categories, social indicators, and data sources in S-LCA

Stakeholders categories	Impact categories	Indicators	References
Workers	Freedom of negotiation and collective association	Cooperation in work-employer relations	WEF (2019a)
		Hiring and firing practices	
	Child labor	Child labor	UNICEF (2019)
		Number of children out of school	
	Fair wage	Minimum wage	ILO (2019)
		Flexibility in determining wages	WEF (2019a)
		Remuneration and productivity	
	Working hours	Average working hours	OCDE (2019)
	Equal opportunity/discrimination	Women's participation in the workforce	WEF (2019b)
		Equal pay for similar work	
	Health and safety	Occurrence of lethal occupational accidents per year	ILO (2019)
		Occurrence of non-lethal occupational accidents per year	
		Workers' exposure to chemicals and contaminants	Regarding the operation of each

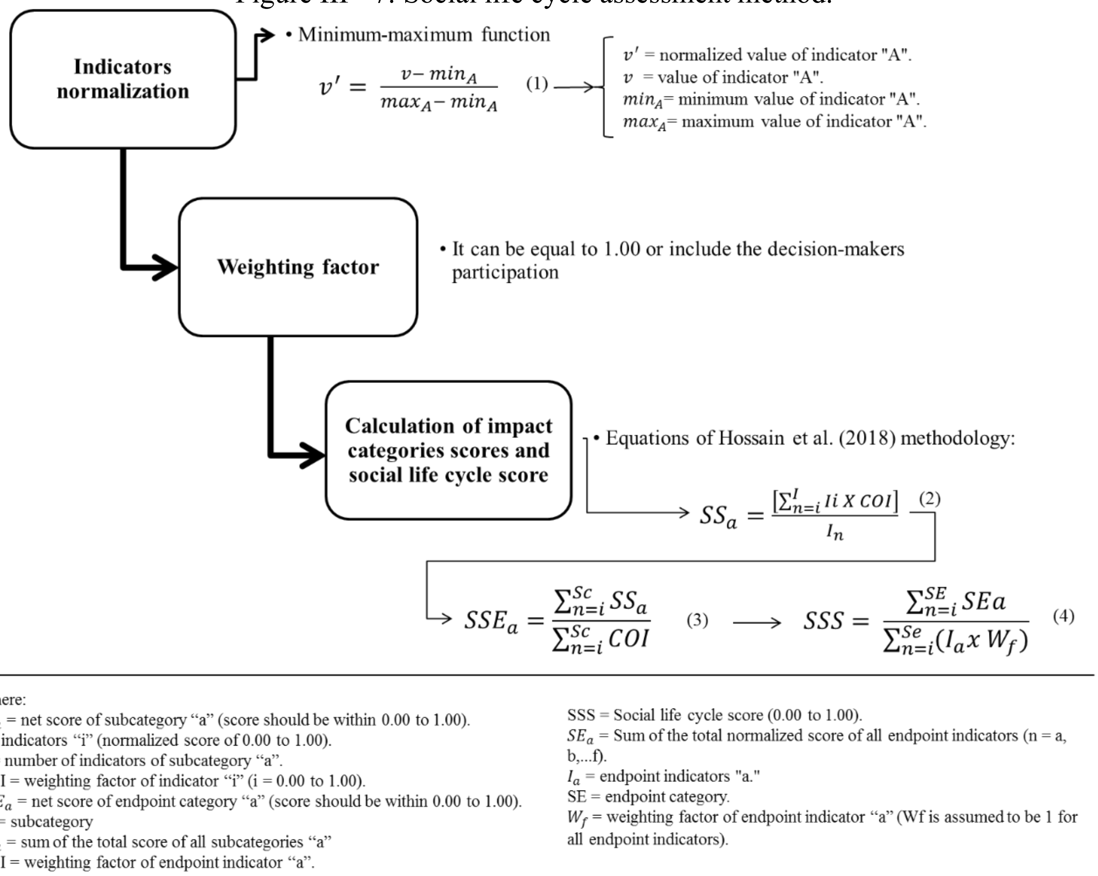
		Generation of hazardous waste and effluents	production method, based on Visentin et al (2021b).
		Health risks during the production process (emission of hazardous gases during production)	
Local Community	Safe and healthy living conditions	Carbon intensity	WEF (2019a)
		Contribution to global warming	Regarding the operation of each production method, based on LCA results.
		Quality of ecosystems	
		Exposure to contaminants (emission of gases that affect human health)	
		Resource usage	
	Access to material resources	Population with access to improved drinking water	WEF (2019a)
		Population with access to improved sanitation	WHO (2019)
		Quality of electricity supply	
Society	Market and work	Country unemployment rate	WEF (2019a)
		Labor market efficiency	
	Contribution to economic development	Extension of marketing	
		Sophistication of the production process	
		Collaboration between university and industry	
	Governance	Efficiency of government spending	
		Transparency in government policy making	
		Total tax rate	
Value chain	Fair competition	Intensity of local competition	
	Promotion of social responsibility	Ability to promote social responsibility	
	Relations with suppliers	Relationship with suppliers	

Social life cycle assessment

The nZVI production methods' social impacts were analyzed using the method of Hossain et al. (2018) and Visentin et al. (2021a). In this method, the social indicators are related to the midpoint and endpoint impact categories, and a social life cycle score is defined. The impact analysis had three stages: normalization of indicators, definition of the weighting factors, and calculation of the impact category and social life cycle scores.

Figure III - 7 shows all the stages of the impact analysis and the equations that were used for such.

Figure III - 7: Social life cycle assessment method.



Initially, the indicators were normalized using the minimum–maximum function (Equation (1)). This standardization aimed to unify all the indicators in the same range of values (from 0.00 to 1.00).

After normalization, the weighting factors of the indicators and midpoint impact categories were defined. In this step, the user can choose to use a weighting factor equal to 1.00 for all the indicators and impact categories, or apply a questionnaire to define different weighting factors on the basis of the decision makers’ opinions. In this work, the weighting factor equal to 1.00 was used. However, in the sensitivity analysis, the sensitivity of the data regarding the use of weighting factors was evaluated on the basis of the experts’ opinion. These weighting factors were obtained from Visentin et al. (2021a).

The third stage of the impact analysis was the calculation of the midpoint and endpoint impact category scores and the social life cycle score using equations (2), (3), and (4), respectively. On the basis of the normalized scores of the indicators and the weighting factor, the score of the midpoint impact category was calculated. The impact score of the endpoint category was calculated on the basis of the score of the midpoint category and the weighting factor of such category. Finally, on the basis of the results of the endpoint category, the social life cycle score was calculated. All social life cycle score calculations were carried out in Excel. The social life cycle score is an adimensional index of values from 0.00 to 1.00; the closer the index is to 1.00 the more socially positive it is.

Table III - 6: Weighting factors for the sustainability index score calculation.

Impact category	Weight
Human health	28.32 %
Ecosystems quality	14.32 %
Local community development	10.24 %
Society development	10.21 %
Climate changes	8.54 %
Environmental external costs	6.53 %
Resources	6.37 %
Management of human resources of a company	5.84 %
Corporate social responsability	5.75 %
Internal costs	3.87 %

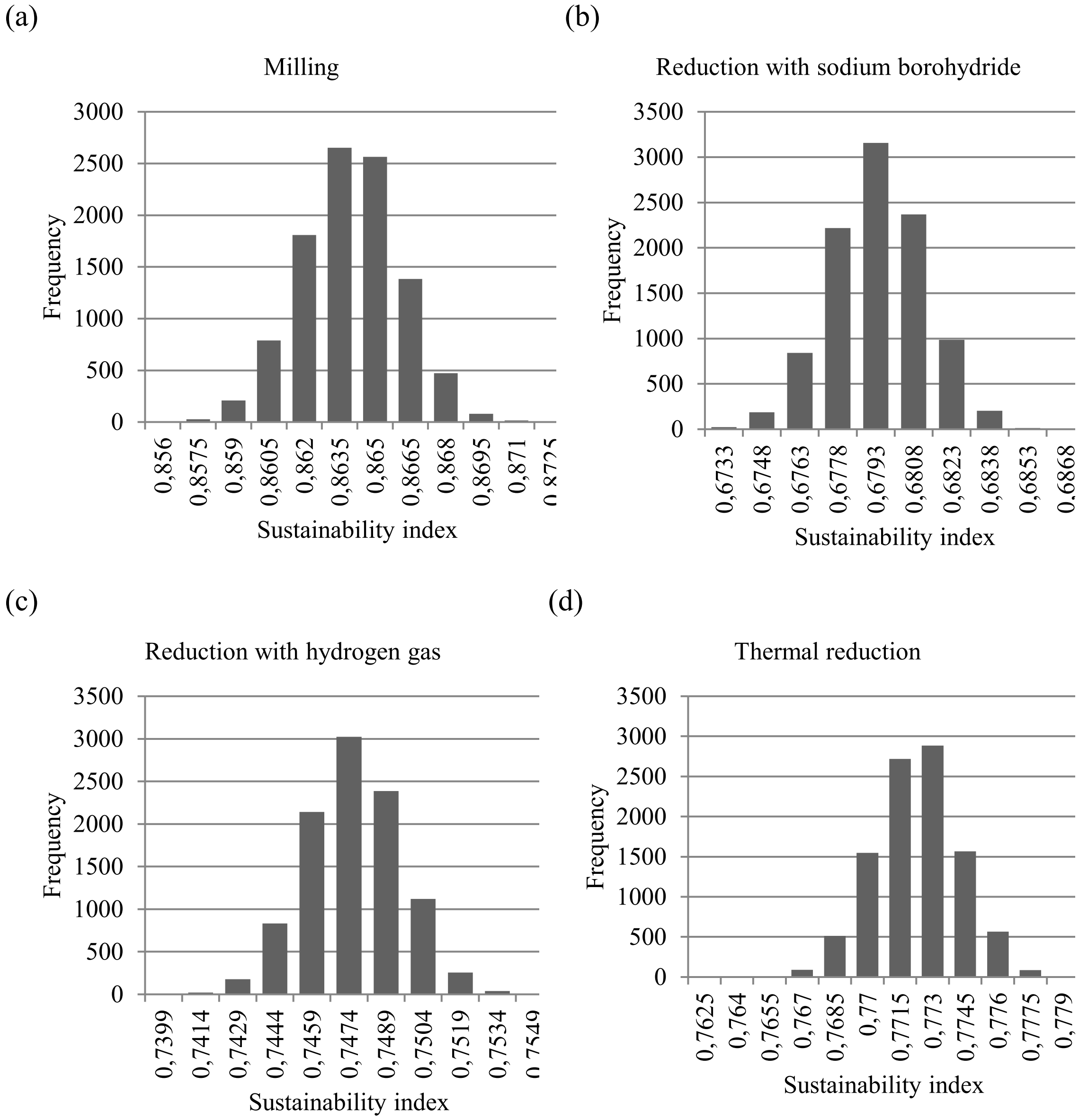
Source: Visentin et al. (2021a).

Table III - 7: Country selection criteria for the sensitivity analysis

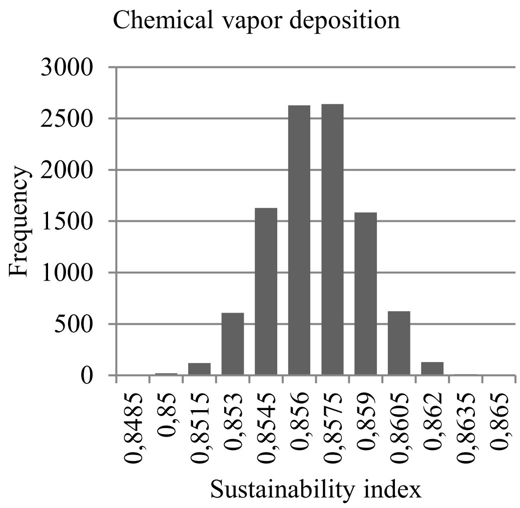
Selection criteria	Selected countries
World large economies	United States, China, Japan, Germany, United Kingdom, India, Brazil, Canada
Social Progress index	Switzerland, Germany, Canada, Japan
Global Sustainability Index	Switzerland, Canada, Germany, United Kingdom
Environmental Performance Index	Switzerland, Germany, Canada, Japan
Countries with higher composition of renewable energy in the energy matrix	Germany, United Kingdom, Brazil, Japan, United States
Countries that publish the most about "soil remediation" (Scopus and Web of Science)	China, United States, United Kingdom, Canada, India, Germany, Brazil, Japan
nZVI production companies	United States, Japan, Czech republic, Canada

Uncertainty analysis

Figure III - 8: Results of the Monte Carlo simulation of the sustainability index values of the nZVI production methods.



(e)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2500
2000
1500
1000
500
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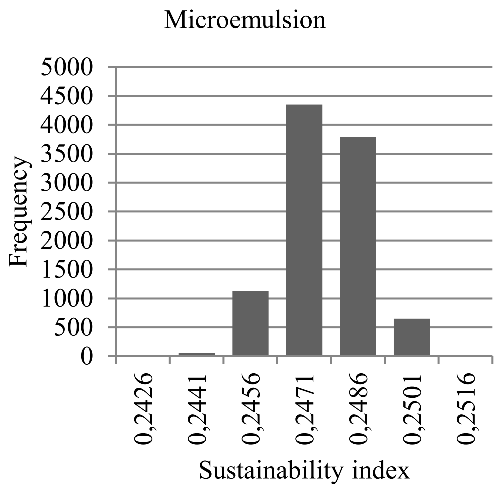
0,85
0,8515
0,853
0,8545
0,856
0,8575
0,859
0,8605
0,862
0,8635
0,865
Sustainability index

(f)


Microemulsion
Frequency
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3500
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2500
2000
1500
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500
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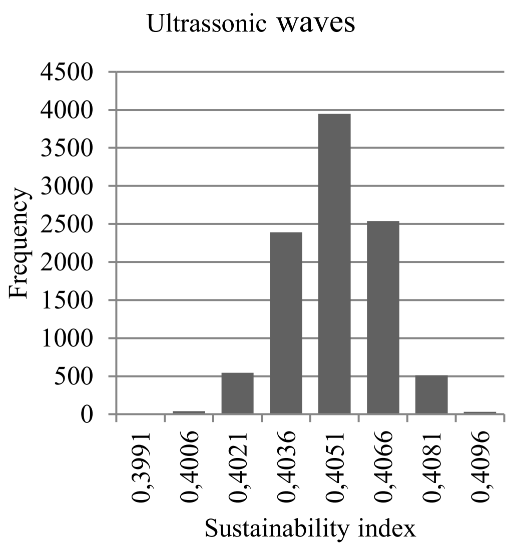
0,2486
0,2501
0,2516
Sustainability index

(g)


Ultrassonic waves
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500
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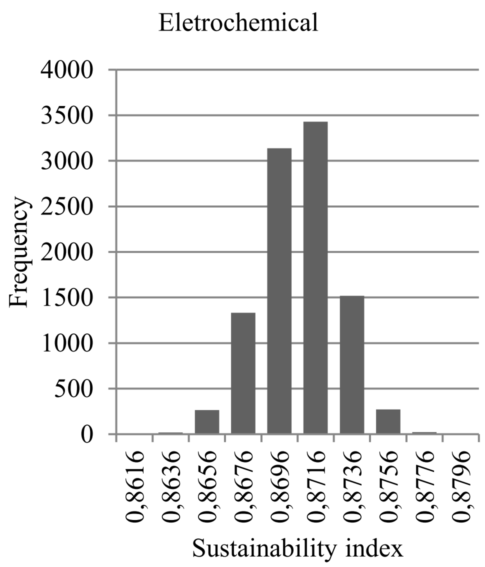
0,4066
0,4081
0,4096
Sustainability index

(h)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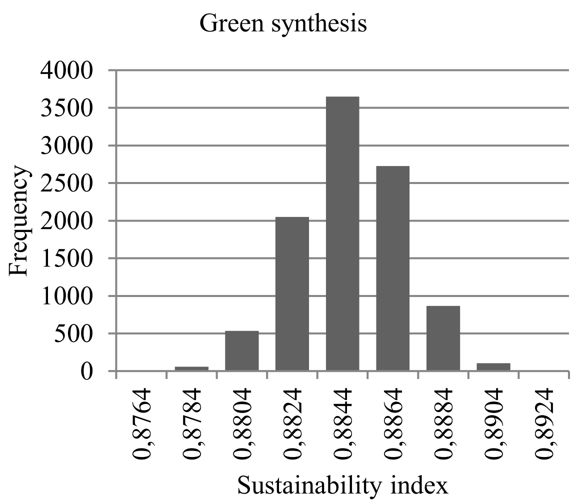
Sustainability index

(i)


Green synthesis
Frequency
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1500
1000
500
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0,8864
0,8884
0,8904
0,8924
Sustainability index

5 CAPÍTULO IV (artigo de resultados – submetido, em revisão): Are contaminated soil and groundwater remediation with nanoscale zero-valent iron sustainable? An analysis of case studies

Abstract: Nanoscale zero valent iron (nZVI) is globally the main nanomaterial used in contaminated site remediation. This study aims to evaluate the sustainability of using nZVI in the nanoremediation of contaminated sites and to determine the factors that affect the sustainability of the use of nZVI in remediation. Five case studies of nZVI use on a pilot scale were selected. Life cycle analysis tools were used to evaluate environmental, economic, and social impacts. Life cycle assessment and life cycle cost analysis were performed in the SimaPro program. The social life cycle assessment was performed in Excel. Life cycle sustainability was determined by multicriteria analysis methods. The functional unit of the life cycle analyses was 1.00 m3 of remediated soil and groundwater. Sensitivity analyses were performed in order to verify the factors that influence the sustainability of using nZVI in remediation. Case study of Brazil was the least sustainable, while case study of United States was the most sustainable. Only the modification of the functional unit results in variations in the sustainability index. Different factors influence the sustainability of nZVI in remediation, the main factor being the amount of nZVI used in the processes. Finally, this work contributes significantly to the state-of-the-art sustainable use of nZVI in remediation. For example, the most sustainable use nZVI in remediation, and also the sustainability of nZVI in remediation is influenced by the amount of nZVI used in remediation, saturation level, soil particle size, permeability, type of contaminant, and location of remediation, among others.

Keywords: sustainable remediation; LCA; LCSA; sustainability; soil saturation; soil particle size.

1. Introduction

The growing interest in nanoremediation in recent years is due to different physical characteristics and chemical properties compared to micro-sized particles, thus causing their use in remediation to be favored (Bardos et al. 2018). For example, iron oxide nanoparticles offer a sorption capacity 10 times greater than microscale particles (Liang and Zhao 2014; Souza et al. 2020). In addition to smaller particle size, nanoparticles also have highly specific surface areas, reactivities, and versatility that give them potential to remove various types of contaminants and achieve the selectivity of target contaminants in complex environmental (Zhang et al., 2019; Qian et al. 2020).

To date, the most widely used nanoparticle in soil and groundwater remediation is nanoscale zero-valent iron (nZVI) due to its low toxicity, high reactivity, and contaminant reduction capacity (Cecchin et al. 2016; Bardos et al. 2018; Blundell and Owens 2020; Shao et al. 2020). nZVI allows for an innovative approach for safe and sustainable remediation of persistent organic compounds such as chlorinated organic contaminants (e.g., solvents, pesticides), halogenated chemicals, and anions or inorganic metals (Mueller et al. 2012; O'Carroll et al. 2013; Chen et al. 2019; Ganie et al. 2021). The use of nZVI for soil and groundwater remediation has been investigated since the late 1990s (O'Carroll et al. 2013). The first field-scale use was in 2000 in the remediation of trichloroethylene in groundwater at a plant in Trenton, New Jersey, USA (Elliott and Zhang 2001). However, according to Bones et al. (2020), few commercial nanoremediation implementations have been carried out so far. Bardos et al. (2018) cite 100 examples of nZVI applications on a pilot and field scale.

Remediation techniques can have both positive and negative environmental, economic, and social impacts. The remediation process is not automatically sustainable, and as such, in recent years, it has been more interesting to consider aspects of sustainability in remediation to balance the benefits with the adverse impacts (Rizzo et al. 2016; O'Connor et al. 2018; Braun et al. 2019). Sustainable remediation is a new approach, which more broadly and holistically considers all the benefits and adverse impacts that may be associated with remediation (Anderson et al. 2018; O'Connor et al. 2018).

One of the tools used in the sustainability analysis of remediation processes is Life Cycle Assessment (LCA) (Visentin et al. 2019a). However, LCA evaluates only the environmental impacts of the life cycle; thus, to assess the sustainability of remediation, it is necessary to use other tools as well, such as Life Cycle Cost (LCC) and Social Life Cycle Assessment (S-LCA) (Kloepffer 2008).

To this end, recent years have seen the advancement of life cycle sustainability analysis (LCSA), which includes environmental, economic, and social aspects (Visentin et al. 2020). The LCSA structure is dependent on three separate lifecycle analysis methods, which have different levels of data availability and maturity. For example, LCA and LCC are widely known and used globally, while S-LCA still has many methodologies that are being developed (Visentin et al. 2020). By contrast, the LCSA structure is globally accepted, and the need for an applicable approach is constantly increasing (Valdivia et al. 2021).

Although the possibility of unique features gives nZVI promise for beneficial applications, it is simultaneously a cause of concern regarding the environmental, economic, and social impacts of its production and use. Some studies have demonstrated the need to evaluate the impacts of nZVI production methods (Martins et al. 2017; Joshi et al. 2018; Visentin et al. 2019b; Visentin et al. 2021a; Visentin et al. 2022). The use of nZVI in remediation is still little explored in relation to impact analysis. To date, only one study has evaluated the sustainability of the use of nZVI in remediation, using data from the NanoRem project carried out by the European Commission's Framework (from 2013 to early 2017) (Bones et al. 2020). Bones et al. (2020) used a NanoRem workbook for sustainability assessment, a process that evaluates sustainability through three stages: preparation, definition, and execution. The evaluation is done qualitatively by defining scores for each sustainability aspect evaluated. Compared to the other techniques evaluated (in situ chemical oxidation, in situ integrated nanoremediation with direct current, and excavation and disposal), nanoremediation was favorable. However, there are still gaps to be filled, and so far, there is no study evaluating the sustainability of the life cycle of using nZVI in the remediation of contaminated sites.

Thus, this study aims to determine the sustainability of the use of nZVI in the nanoremediation of contaminated sites through the analysis of different case studies. The specific objectives are (i) to verify the variability of sustainability considering different case studies with different nZVI usage configurations in the application of nanoremediation of contaminated sites, soil, or groundwater; (ii) to analyze the sensitivity of sustainability considering different variations; and (iii) to determine the factors that influence the sustainability of the use of nZVI in the remediation of contaminated sites.

2. Methodology

2.1 Case study descriptions

For impact analysis, five case studies were considered (Table 1). The studies were selected through a search of several databases (Scopus, Web of Science, Google Scholar) through the use of keywords such as "remediation," "nanoremediation," "nano scale zero valent iron," "nZVI," and "pilot scale."

The selected studies correspond to different practical uses of nZVI on pilot, field, and laboratory scales in different locations around the world. The studies include in situ remediation of soils (unsaturated) and groundwater (saturated soils), covering different types of soils and contaminants.

For contaminated site remediation with nZVI there is no standard application, for example, in relation to the concentration of nZVI or injection time, so bench tests are essential. Furthermore, the variations in application observed in the case studies seek to evaluate more comprehensively the life cycle impacts of the use of nZVI. Table IV - 1 illustrates an overview of the case studies considered, detailing the soil condition (saturated/unsaturated), soil type, contaminant and concentration, remediation efficiency, nZVI concentration, injection process, and monitoring. More detailed information can be found in the Supplementary Material.

Table IV - 1: Parameters of case studies of life cycle analyses.

Parameters	**Case study 01 Vanzetto and Thomé (2022)**	**Case study 02 Zhang et al. (2018)**	**Case study 03 Otaegi and Cagigal (2017)**	**Case study 04 Laszlo and Szabo (2017)**	**Case study 05 He et al. (2010)**
Remediation scale	Pilot scale/laboratory	Pilot scale/laboratory	Lab scale – NanoRem project	Lab scale – NanoRem project	Pilot scale/laboratory
Soil saturation level	Unsaturated	Unsaturated	Saturated	Saturated	Saturated
Soil type	Oxisoil 72% clay 15% silt 3% sand	Sandy soil 59% sand 22.5% silt 18.5% clay	Sandy gravel with boulders	Sandy gravel (with layers of sandy gravel, silty clay and holocene sand)	Mixture of silt, siliceous limestone fragments and a small clay fraction
Hydraulic conductivity	$1.3x10^{-3}$ cm/s	$5.3x10^{-4}$ cm/s	$5.7x10^{-4}$ cm/s	$7.6x10^{-2}$ cm/s	$1.9x10^{-3}$ cm/s
Remediation volume of soil/groundwater	0.2 m^3	1.00 kg of soil	28,904 m^3	190,000 m^3.	64.10 m^3.
Type of contaminant and concentration	Hexavalent chromium (100 mg/kg) and pentachlorophenol (100 mg/kg)	Hexavalent chromium (800 mg/kg)	Arsenic (5527 µg/L)	Chlorinated hydrocarbons (15-20,000 µg/L)	PCE = 1.20 – 12.0 mg/L, TCE = 1.6–23.8 mg/L, cis-DCE = 8.5–20 mg/L, VC = 1.1–2.2 mg/L and PCB1242 = 6.9– 97.4 µg/L.

Parameters	Case study 01 Vanzetto and Thomé (2022)	Case study 02 Zhang et al. (2018)	Case study 03 Otaegi and Cagigal (2017)	Case study 04 Laszlo and Szabo (2017)	Case study 05 He et al. (2010)
Intervention value	In Brazil, for Cr (VI) is 0.4 mg/kg and pentachlorophenol 0.16 mg/kg	In China, for Cr (VI) is 5 mg/kg (Sun et al. 2019).	The Dutch intervention value of Arsenic is 60 µg/l.	The Dutch intervention value of chlorinated hydrocarbons is 10 µg/l.	The USEPA intervention value of PCE/TCE/DCE /PCB are 14 µg/l.
nZVI concentration	40 g/kg	11 mg/kg	10 g/L	10 g/L	0.2 g/L and 10 g/L
Injection process and monitoring	The injection was performed at one point, with the injection pressure of 90 psi lasting 6 minutes, with an injection rate of 2 L/min. A total of 4.39 kg of nZVI were injected. The nZVI used was nanofer star from NanoIron located in the Czech Republic. Before the injection of nZVI, activation was made with water and agitation according to the manufacturer's guidance. The monitoring was carried out in twenty points, collecting samples at 8 different times during the period of 120 days.	The injection was performed at one point, under pressure, with a rate of 0.05 L/min. The nZVI-CMC used in the study was synthesized on site using the chemical reduction method with sodium borohydride. The monitoring was carried out in twenty points, collecting samples at 8 different times during the period of 120 days.	The injection occurred in three injection points in a triangular configuration, low pressure (< 5bar) and a flow rate of approximately 0.6 - 1m³/hour. A total of 250 kg of nZVI was injected into the pilot area. The nZVI used was nanofer star from NanoIron located in the Czech Republic. Before the injection of nZVI, activation was made with water and agitation according to the manufacturer's guidance. Monitoring was performed through eight monitoring wells and was performed in 28 days, from the day of injection to six months after remediation.	Injection under pressure. The nZVI used for remediation was provided by ScIDre GmbH from Dresden, Germany. Before remediation the suspension was prepared, mixing the nZVI with oxygen-free water using tanks. The suspension was pumped from the tanks to the injection well used a hydraulic pump. The injection occurred under pressure of 0.5 to 5 bar in three injection wells, at a rate of 20 – 30 L/min. A whole, 176.8 kg of nZVI were injected. Monitoring was carried out in 14 wells, in 8 days of monitoring during the period of -5 to 360 days.	Injection in two stages: gravity and under pressure. The first injection was performed using a peristaltic pump to transport the nZVI suspension from the tank to the injection well, the pump did not exert injection pressure. The injection rate was 2.54 L/min, and lasted 3.7 hours. The second injection occurred under pressure, and in this case the pump exerted injection pressure, which was less than 0.35 bar. The injection rate was 5 L/min and lasted 1.8 hours. The nZVI used in remediation was produced on site using the chemical reduction method with sodium borohydride. In the first injection, 114 g of nZVI was used at a concentration of 0.2 g/L, while

					in the second injection they were 569 g at a concentration of 10 g/L. The monitoring was carried out in three wells, in 20 days of monitoring during the period from 0 to 600 days.
Remediation efficiency	83%	95%	> 90%	> 60%	> 90%
Remediation location	Brazil	China	Spain	Hungary	United States

2.2 Life cycle sustainability assessment

In this study, LCA (environmental), LCC (economic), S-LCA (social), and LCSA (sustainability) were performed. The analyses were performed based on ISO 14040 (2006), which defines the stages of life cycle analysis as the definition of objective and scope, inventory analysis, impact assessment, and interpretation. In the sequence are detailed the methodological procedures of each step.

2.1.1 Goal and scope definition

The goal of life cycle analyses is to evaluate the environmental, economic, social and sustainability impacts of the life cycle of nZVI use on the environmental remediation of soils and groundwater. The intended application of the analyses is to verify whether the sustainability of nZVI can be influenced by the different practical uses of the selected case studies. The target audience is researchers in the field of sustainable remediation and decision makers.

The scope of this work includes a “cradle-to-grave” approach. The limits of the system involve the stages of raw material extraction and nZVI production, transportation, and use in nanoremediation of contaminated sites. In the case of in situ remediation, there is no removal of nZVI from the soil or groundwater after the remediation process, so the end of the life cycle of nZVI is its application in situ. In the case of in in situ remediation, nZVI particles are adhered to soil particles and are not removed or discarded. Ex situ remediation of nZVI is not applied in practice as in these cases other technologies are more viable. The functional unit of LCA is the remediation of 1.00 m^3 of soil or groundwater.

In this work, an attributional LCA was developed with the objective of describing the environmentally relevant physical flows of the life cycle of nZVI and its subsystems. In LCC, only processes within the system limit that impose economic costs, especially direct costs, are considered for analysis. In addition, external environmental costs, such as carbon emissions, are also included (Visentin et al. 2021a).

2.1.2 Inventory analysis

All inventory data were secondary, obtained directly from the reference publications of each case study and through estimates considering studies with similar processes. Another source of inventory data was the Ecoinvent database (version 3.6). Ecoinvent data were selected considering the allocation model at the point of substitution (Ekvall 2019). The geographic locations of the data were selected, when possible, considering the data of the countries of location of the case studies (01 Brazil, 02 China, 03 Spain, 04 Hungary, and 05 United States). In data for which there was no availability of geographic location selection, the geographical location "rest-of-world" was considered. This location considers an overall location average of the data for a given product. In this type of location, uncertainty is considered, through the residual difference between the global dataset and the non-global datasets, when all datasets are scaled to the production volume of the reference product.

For LCC, data were obtained from companies providing services used in remediation, such as excavation, transportation, injection equipment, labor, disposal of solid waste, and effluent treatment of each country. The social data used were at the country level, obtained from worldwide reports from organizations such as the World Economic Forum, the International Labor Organization, the World Health Organization, the Organization for Economic Co-operation and Development, and the United Nations International Children's Emergency Fund.

In S-LCA, data collection was structured through a set of indicators associated with impact categories and stakeholders. These sets of factors were determined prior to the application of the analysis through a systematic review in the publications referring to S-LCA. Thus, five categories of stakeholders were selected: workers, consumers, local communities, society, and value chain; this yielded 19 impact categories and 37 indicators. All inventory data are presented in the Supplementary Material.

2.1.3 Impact assessment

The analysis of impacts differs in each of the LCAs regarding the computational programs and the methods of analysis used. Thus, for a better understanding of the impact assessment methodology, the methodological procedures of each LCA are presented in separate sections.

Life Cycle Assessment

LCA was carried out in the SimaPro program, version 9.1.1.7. The impact analysis method used was impact 2002+ because this method is used in most studies of LCA and nanomaterials and it has already been used in previous studies by Visentin et al. (2019b, 2021a). The categories of endpoint impact evaluated were human health, ecosystem quality, climate change, and resources. In addition, mid-point impact categories were also considered in the LCC.

Life Cycle Cost

LCC was performed in SimaPro through the elaboration of a cost analysis method as detailed in previous studies by Visentin et al. (2019b, 2021a) and Banar and Özdemir (2015). SimaPro does not have a cost analysis method, so by designing a cost method, one can use the data already defined in the LCA to add the cost component to LCA inventory. The procedure is the same as that used in SimaPro for LCA; however, the cost method created is selected at the time of impact analysis.

The cost categories evaluated were the internal costs directly related to the use of nZVI (raw materials, energy, fuels, labor costs, etc.) and also the external costs that correspond to the environmental costs related to the environmental impacts resulting from the use of nZVI. The external costs considered were global warming (kg CO2 eq), eutrophication (kg PO4 P-lim), acidification (kg SO2 eq), depletion of the ozone layer (kg CFC-11 eq), photochemical oxidation (kg C2H4 eq), and inorganic respiratory diseases (kg PM2.5 eq). External costs were quantified according to values obtained by Visentin et al. (2019b).

Because the inventory data were secondary, a Monte Carlo analysis was performed on the LCC results obtained from SimaPro in order to minimize uncertainties. For this, the initial costs (external and internal) resulting from the application of the LCC were analyzed, through 10,000 times the total Monte Carlo simulation, with a probability (p-value) of 0.80. In this type of study, it is very difficult to estimate costs with precision, so the p-value used is justified (Wang, Chang, and El-Sheikh, 2012; Visentin et al. 2021a). After applying the method, the average value of the attempts were set to the lifecycle cost value. Final costs are presented in US dollars ($).

Social Life Cycle Assessment

The S-LCA was performed according to the methodology detailed by Visentin et al. (2021c) based on the methodology of Hossain et al. (2018). This methodology is based on equations to determine the impacts of midpoints and endpoints in the categories of stakeholders considered: workers, consumers, local community, value chain, and society.

Initially, social inventory data should be normalized for common units using the minimum-maximum equation after equations are applied that relate the normalized score of social indicators with weighting factors for the calculation of the impacts of point method and endpoint. Finally, a social life cycle score is calculated. In this study, the participation of stakeholders in the definition of weighting factors was not considered because, as detailed by Visentin et al. (2021a), there are no significant differences in the results of the social life cycle score with the participation of stakeholders in relation to weighting factors with equal weights.

Life Cycle Sustainability Assessment

LCSA was determined by a multicriteria analysis method according to the methodology of Visentin et al. (2021a). LCSA is based on the results of previously performed life cycle analyses (LCA, LCC, and S-LCA) in the endpoint impact categories. The scores in the endpoint impact categories are used because it is possible to perform a more comprehensive analysis than if only the environmental, economic, and social results as a whole are considered.

The initial LCSA methodology entails the normalization of the results of LCA using the minimum-maximum normalization equation. Then, analyses can be made with specialists to determine the weighting factors. In this study, the participation of experts was not considered because in Visentin et al. (2021a) it was verified that there are no significant differences in the results. However, it is noteworthy that the participation of stakeholders is a fundamental process for the results to reflect on the reality of the agents involved. Finally, the sustainability index is calculated through a multi-attribute method that considers the normalized score of each impact category with weighting factors. The sustainability index results in a score from 0.00 to 1.00 and is classified as initially presented in Hossain et al. (2018) and adapted in Visentin et al. (2021a): highly unsustainable (0.00 to 0.20), unsustainable (0.21 to 0.40), neutral (0.41 to 0.60), sustainable (0.61 to 0.80), and highly sustainable (0.81 to 1.00).

2.1.3.1 Sensitivity analysis

Sensitivity analysis seeks to demonstrate the sensitivity of the results according to changes in the parameters of the analysis. For this study, sensitivity analysis was performed in individual LCAs (environmental, economic, and social) and also in the sustainability analysis considering the variation of five factors.

(i) *Modification in injection configuration: pressure injection (initial scenario) and gravity injection.* In this analysis, injection by gravity is considered, thus excluding the injection pump and including only the pressurizer that is used to move the nZVI to the injection well. In addition, injection time was considered twice as long in all case studies, according to He et al. (2010).

(ii) *Use of other materials in injection and monitoring tubes (e.g., reuse/recycling, polyethylene, steel, aluminum, and iron pipes).* In all case studies, PVC pipes were initially considered for injection wells and monitoring, though other materials can also be used.

(iii) *Synthesis of nZVI at the site of remediation considering the nine production methods detailed in Visentin et al. (2021b) (milling, sodium borohydride reduction, hydrogen gas reduction, hot reduction, vapor deposition, microemulsion, ultrasonic waves, electrochemical, and green synthesis).* In this analysis, only the production method of the nZVI used was made, which was performed on site. The amount of nZVI used in the initial studies was maintained, and the variation was not considered a function of the difference in efficiency that may have resulted from the different characteristics of the nZVI produced by each method. This variation seeks to verify whether the on-site production by different methods and the absence of transport of the nZVI have an influence on the sustainability index. Through the production on the site of nZVI, no impacts were found related to the transport of nZVI from the place of marketing to the place of remediation.

(iv) *Considering the use of nZVI from different supplier companies worldwide, including Nanoiron s.r.o. (Czech Republic), All Kogyo Corp. (Japan), NanoAmor, Amorphous Products (United States), Golder Associates Inc. (United States), and Scientific Instruments Dresden GmbH (Germany).* As detailed by Visentin et al. (2021b), the companies that sell nZVI use different production methods, which result in variations in terms of environmental and social impacts and costs, and consequently sustainability. Thus, this variation aimed to verify whether the sustainability index varies if the purchase of nZVI from different companies is considered, in addition to the transport resulting from the place of marketing until the remeasurement.

(v) *Modification of the functional LCA unit of 1.00 m³ of soil and groundwater remediated to 1.00 kg of nZVI.* This variation aims to verify whether the amount of nZVI has a direct influence on the sustainability index of the case studies.

3 Results and Discussion

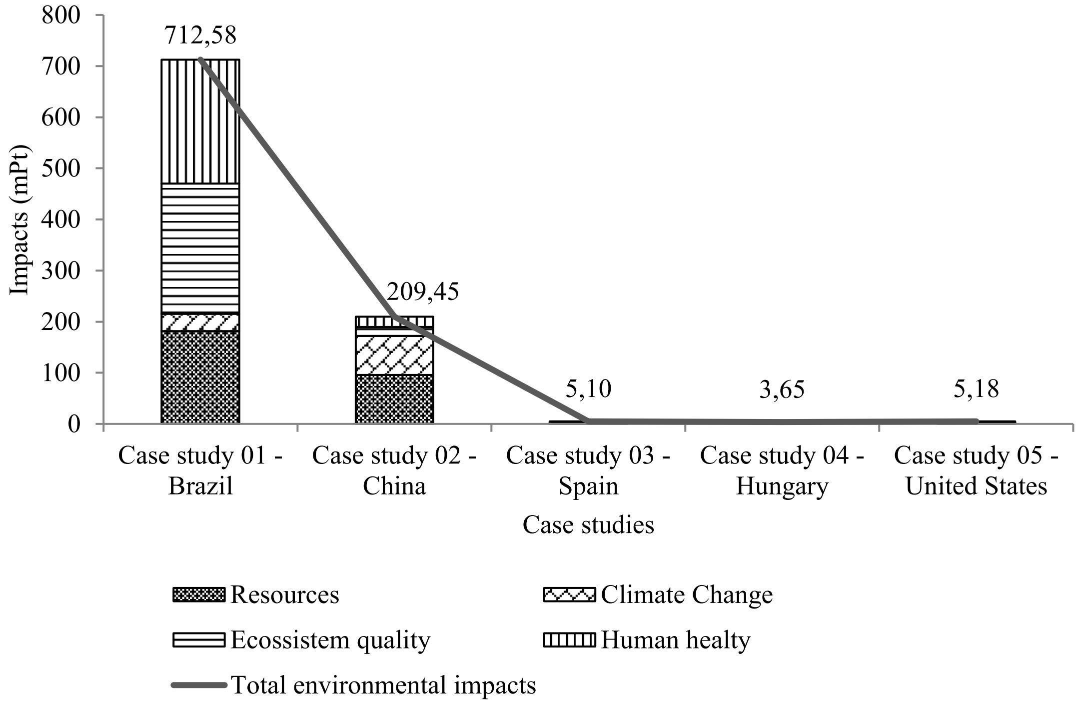
3.1 Life cycle assessment

Figure IV - 1 (a) presents the results of the LCA regarding the total environmental impacts of the case studies analyzed in the impact categories, and (b) presents the results of case studies 03 Spain, 04 Hungary, and 05 United States, (c) details the percentage impacts at each stage of the lifecycle.

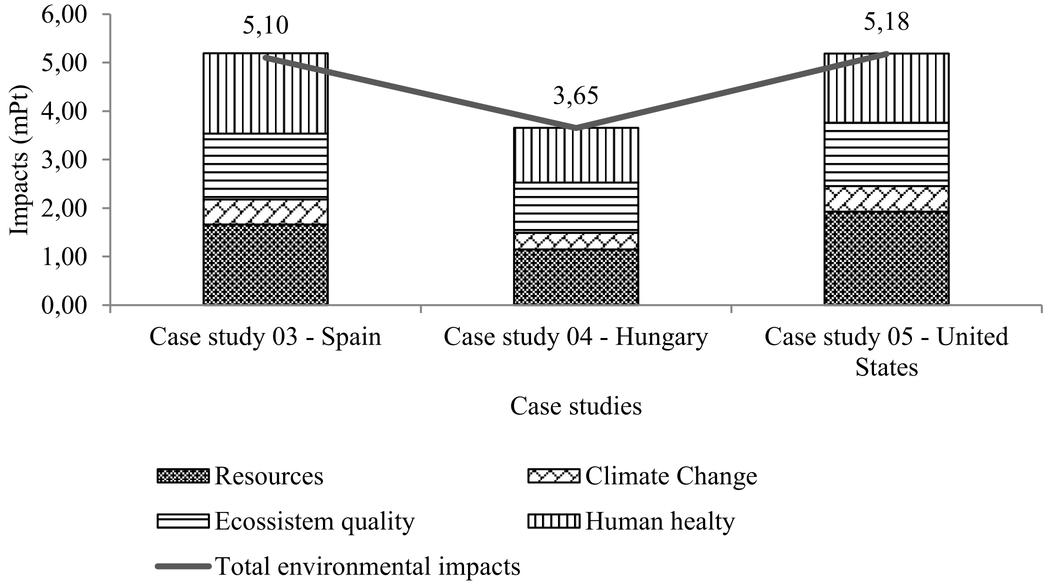
The results of the environmental impacts are expressed in mPt (millionths of a point). The magnitude of this numerical value expresses the size of the global environmental impact; that is, the higher the value of the indicator, the greater the environmental impact of the method (Visentin et al. 2019b). In all case studies, the disposal of solid waste in hazardous waste landfills and the treatment of effluence through industrial effluent treatment plants was considered.

Figure IV - 1: (a) Total environmental impacts of case studies and the impact categories of 1.00 m³ of soil and groundwater remediated. (b) Environmental impacts of case studies 03 Spain, 04 Hungary, and 05 United States on impact categories. (c) Contribution of each stage of the life cycle to the environmental impacts of case studies in terms of percentage.

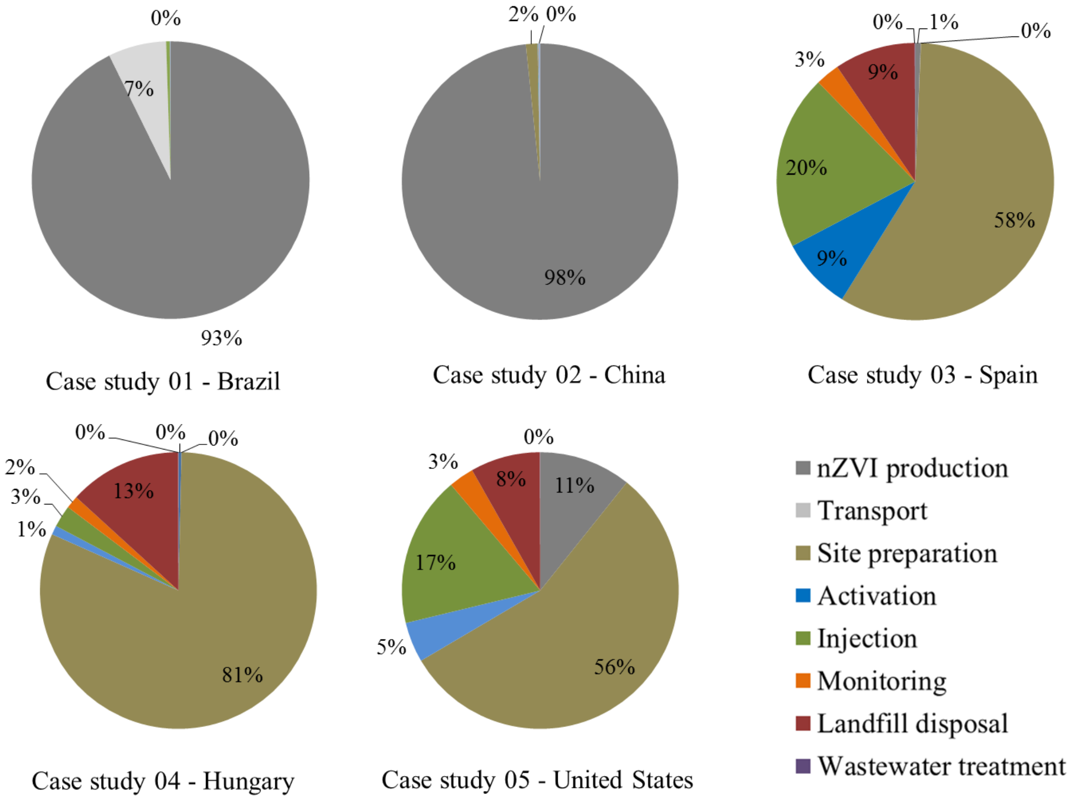
(a)



(b)



(c)



Overall, case study 01 Brazil, which refers to the remediation of an unsaturated Oxisoil contaminated with chromium and PCP, resulted in the greatest environmental impacts of all the cases analyzed. The impacts of this case mainly refer to the production of nZVI (93.00%), which for this study corresponded to 21.95 kg for the remediation of 1.00 m^3 of contaminated soil. In addition, transport also contributes to the impacts of the method. The other steps resulted in minimal contributions to the impacts of this case study.

Then, case study 02 China, referring to the remediation of unsaturated soil composed of sand, silt, and clay contaminated with Cr (VI), resulted in the second largest impact of the life cycle of the evaluated studies. The impacts of case study 02 China mainly refer to the production of nZVI (98.35%); similar to case study 01 Brazil, case study 02 China used a high amount of nZVI, 13.31 kg for the remediation of 1.00 m^3 of contaminated soil. Site preparation contributed to 1.4% of the impacts of the study, while the other steps resulted in minimal contributions to impacts.

The other case studies (03 Spain, 04 Hungary, and 05 United States) refer to the remediation of different types of saturated soils with different contaminants. Case study 05 United States refers to the remediation of soil with a mixture of silt, fragments of siliceous limestone gravel, and clay contaminated with organic compounds, resulting in the greatest impacts of all the case studies of saturated soils. In this case study, nZVI is produced at the site of the nZVI through the sodium borohydride reduction method, which contributes to 10.74% of the impacts of the study. Moreover, in this case, the amount of nZVI used is higher in relation to other case studies of saturated soil, due to the use of two injections of nZVI and to the soil characteristics of thinner grains such as silt and clay. The preparation of the site, which involves the activities of digging wells and the use of PVC, makes the greatest contribution to the impacts of the study at 55.8%. The injection stage contributes to 17.6% of the impacts of the study, which refers to the energy consumption by the injection equipment.

Case study 03 Spain, referring to the remediation of soil with sandy gravel and saturated boulders contaminated with arsenic, resulted in the third largest impact out of the case studies with saturated soils. Regarding the stages of the life cycle, the greatest contribution of impacts occurs in the stages of site preparation and injection. The preparation of the site involves the activities of digging the monitoring wells, transporting equipment and waste, and using PVC for the wells. The injection step involves energy consumption by the pumps used in the process. In this case, the injection time of nZVI is the largest compared to the other case studies of saturated soils because the hydraulic conductivity of the soil is the lowest compared to the other case studies ($5.7x10^{-4}$ cm/s). Thus, a longer injection time is required for the nZVI particles to be distributed, and the energy consumption in this method is higher.

Case study 04 Hungary resulted in the lowest environmental impacts of the analyzed studies. In this case, soil with layers of sandy gravel, silt, clay, and sand contaminated with organic compounds was remediated. The greatest impacts were verified in the site preparation stage, at 81.3%. The injection stage contributed 2.5% of the impacts because, in this case, the injection time of the nZVI was the lowest verified in the case studies of saturated soil. This is justified due to the greater hydraulic conductivity of the soil ($7.6x10^{-2}$ cm/s).

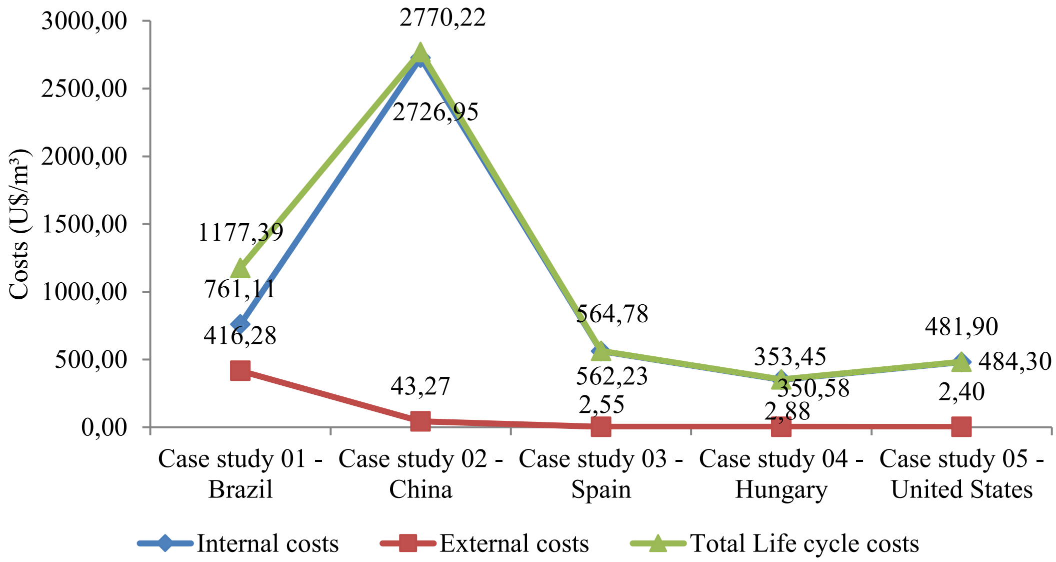
Thus, in general, it is perceived that the environmental impacts of the use of nZVI are related: the amount of nZVI used and the impacts of the production of the nZVI, as well as the processes involved in the preparation of the site for remediation (excavation, transport, disposal of waste, and materials used, such as PVC) and injection time. To improve the environmental aspects of the use of nZVI, some alternatives can be considered, such as production at the nZVI site by more sustainable methods (Visentin et al. 2022), nZVI gravity injection, and the use of other materials for injection tubes and monitoring.

3.2 Life cycle cost

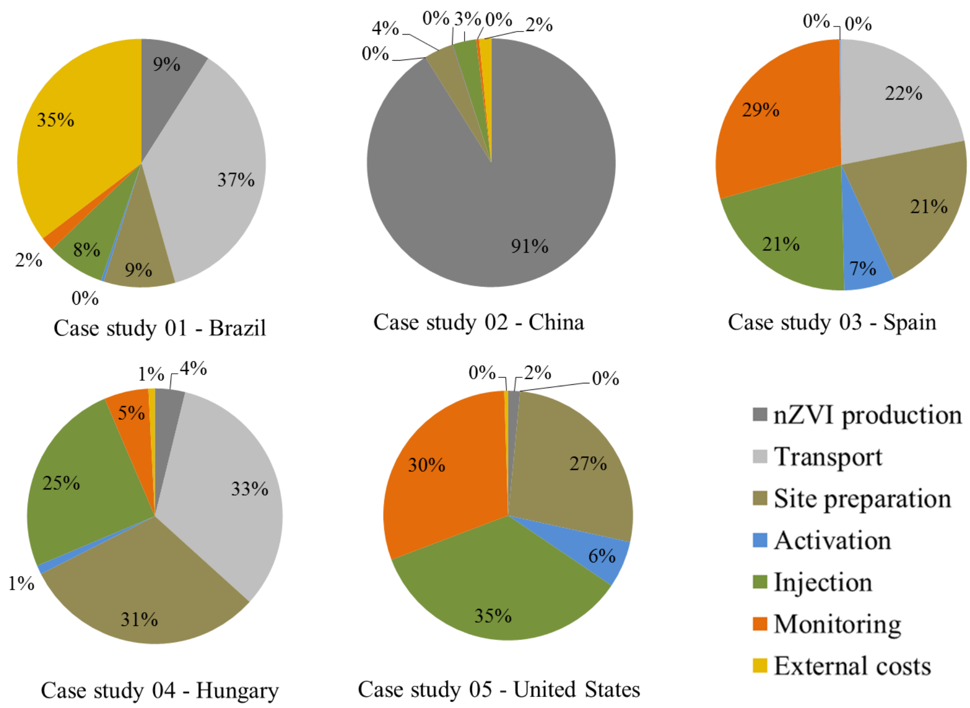
Figure IV - 2 (a) presents the results of the LCC regarding the total life cycle costs of the analyzed case studies, (b) details the costs in terms of percentage at each stage of the lifecycle. The costs are expressed in US $ per m³. All cost components were selected according to the locations of the case studies, so the labor costs, for example, are those applied in each case study location.

Figure IV - 2: (a) Life cycle of case studies and in the costs categories. (b) Contribution of each stage of the life cycle to the costs of case studies in terms of percentage.

(a)



(b)



Case study 02 China resulted in the highest life cycle costs of all case studies at U$2,726/m³. The highest costs were associated with the production of nZVI-CMC, which uses expensive reagents such as sodium borohydride and iron sulfate. In addition, the amount of nZVI-CMC used also contributed to the costs. The other steps resulted in 9.00% of the life cycle costs.

Case study 01 Brazil resulted in the second highest cost of the life cycle of all case studies at U$1,177.39/m³. This is justified because case study 01 Brazil uses the largest amount of nZVI of all the case studies. The steps of external costs and transportation contributed most to the life cycle costs of case study 01 Brazil.

Case study 03 Spain resulted in the third highest cost of the life cycle of the studies analyzed, coming in at U$565.63/m³. The main components affecting the costs of the method were the labor costs in the monitoring step, in addition to transportation, site preparation, and injection. External costs were low due to the low environmental impact of the method, as detailed earlier.

Case study 05 United States resulted in life cycle costs of U$484.82/m³. In this case, there was production at the nZVI site and thus no transport of the nZVI. The main steps that contributed to the costs of the study were site preparation, injection, and monitoring. In these steps, labor costs contributed significantly to overall costs.

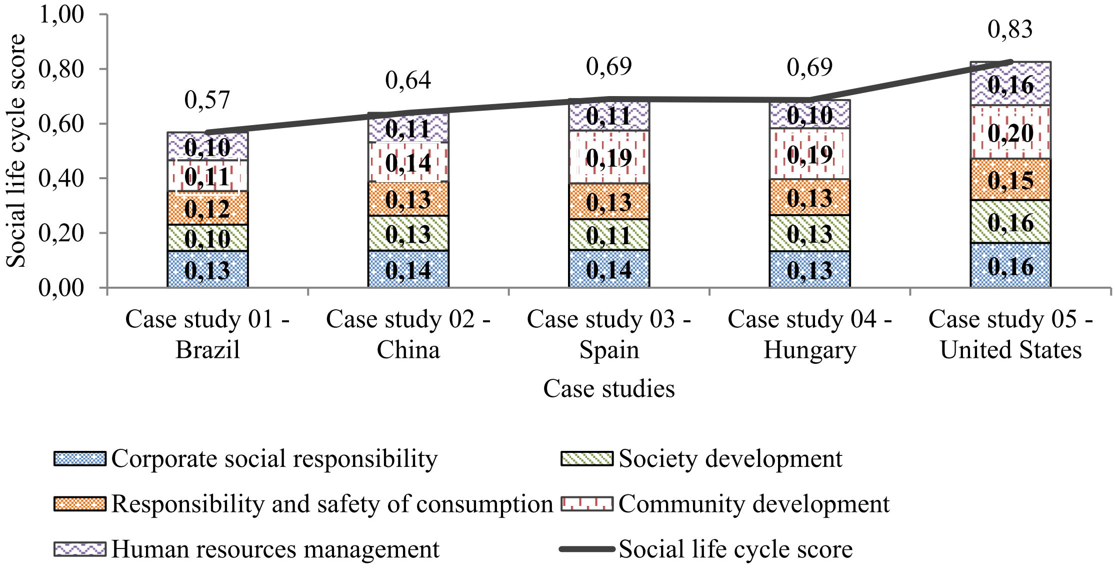
Case study 04 Hungary resulted in the lowest life cycle costs at $354.13/m³. The main steps that contributed to the costs of the case were transportation, site preparation, and injection. Preparation of the site included the PVC pipes that are used in the injection, the labor costs for the preparation of the site with the placement of the pipes, and the transport of the machinery.

Thus, it is perceived that in general the costs of using nZVI are dependent on the transport costs of nZVI, site preparation methods, the tubes used for injection and monitoring, and the labor costs for each site. Different configurations can influence costs, such as on-site production of nZVI, buying from other companies to lower transport costs, and using other types of pipes.

3.3 Social life cycle assessment

Figure IV - 3 presents the results of the total social life cycle scores and the impact categories evaluated. The social life cycle scores are expressed as dimensionless scores of 0.00 to 1.00, with values close to 0.00 showing a worse social classification and values close to 1.00 showing a better social classification.

Figure IV - 3: Total social life cycle scores and scores in social impact categories.



Case study 01 Brazil resulted in the lowest social life cycle score, followed by case study 02 China. The social life cycle scores of case studies 03 Spain and 04 Hungary were equal in the middle, while case study 05 United States had the highest social life cycle score.

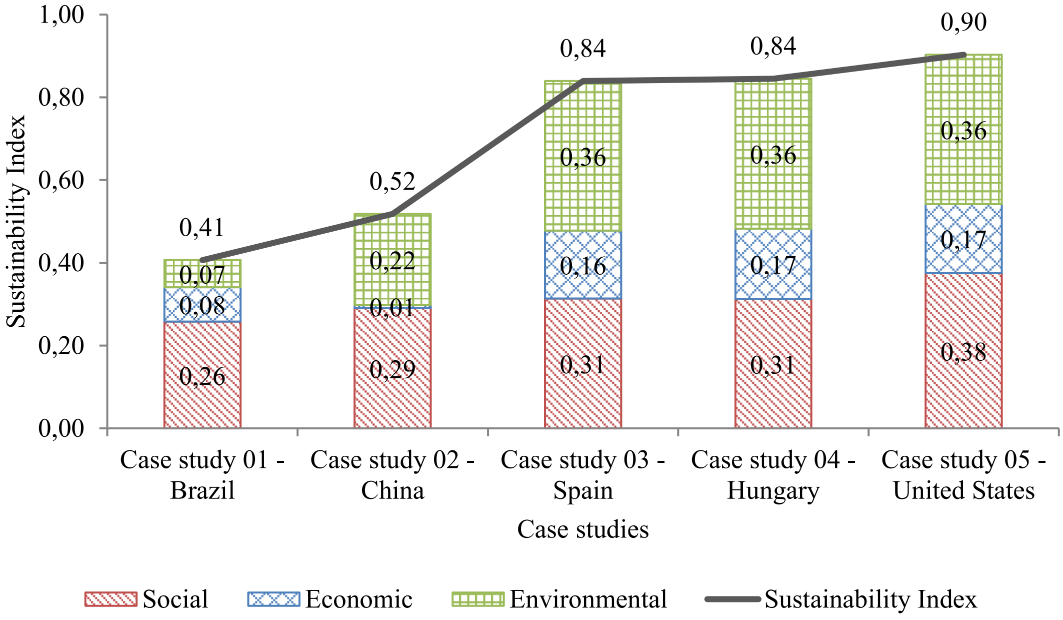
In the impact categories, the maximum score allowed is 0.20 because the social life cycle score is a sum of the scores of each category. Case study 05 United States resulted in the highest social life cycle score in all categories evaluated. By contrast, case study 01 Brazil resulted in the lowest scores in the impact categories.

As detailed in the methodology, the S-LCA was carried out with inventory data at the country level because using data at the sector level or obtained directly from companies is not possible, due to industrial privacy. Case studies 01 Brazil and 02 China refer to developing countries, which in many indicators have lower scores compared to developed countries, such as other case studies (03 Spain and 04 Hungary). This is especially true when compared to case study 05 United States. Visentin et al. (2021c) demonstrated the variability of the social life cycle score according to the indicator data countries considered, noting that, for example, considering data from the United Kingdom and Switzerland, the social life cycle scores were highest compared to Brazil.

3.4 Life cycle sustainability assessment

Figure IV - 4 presents the sustainability index of the case studies evaluated. The sustainability index is a dimensional index of 0.00 to 1.00, with values closer to 1.00 being more highly sustainable. The classification of the sustainability index used in this study was previously detailed in section 2.2.3.

Figure IV - 4: Sustainability index of case studies.



Case study 05 United States resulted in the highest sustainability index of all the studies evaluated, followed by case studies 04 Hungary and 03 Spain. The sustainability indexes of these case studies is classified as highly sustainable. Case study 01 Brazil resulted in the lowest sustainability index of all the case studies evaluated, followed by the case study 02 China. Case studies 01 Brazil and 02 China are classified as neutral, the other case studies are classified as highly sustainable

Sustainability is related to the amount of nZVI used in remediation. Case studies 01 Brazil and 02 China, which use high amounts of nZVI for the remediation of 1.00 m³ of contaminated soil (21.95 kg and 13.31 kg, respectively), were the ones that obtained the lowest sustainability indexes. In addition, these case studies also resulted in higher environmental impacts, higher costs, and lower social life cycle scores. On the other hand, the other case studies that used smaller amounts of nZVI (e.g., 10.62 g in case study 05 United States) resulted in the highest sustainability indexes. A detailed analysis of the factors that influence the sustainability of the nZVI life cycle is presented in section 3.5.

LCSA is based on the results of life cycle analyses previously presented in the endpoint impact categories, using an equal weighting factor for all impact categories and not considering stakeholder participation. According to Visentin et al. (2021a), the participation of stakeholders in the definition of weights does not result in significant variations in the sustainability index compared to the use of equal weighting factors. However, it is noteworthy that the participation of stakeholders is fundamental in situations for which we want to obtain a representative result of a given situation (Søndergaard and Owsianiak 2018).

3.4.1 Sensitivity analysis

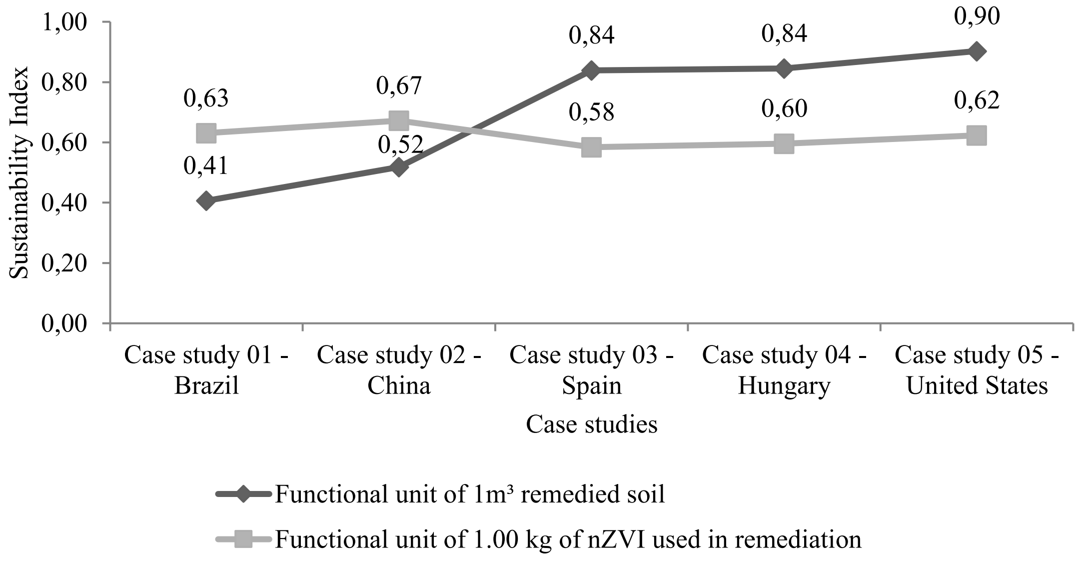
Table IV - 2 presents the results of the sustainability index of sensitivity analyses performed (variations *i* to *iv*), except for the analysis of the variation of the functional unit (variation *v* of sensitivity analyses), which is presented in Figure IV - 5. The sensitivity analysis of the sustainability index incorporates the results of sensitivity analyses of individual life cycle analyses (LCA, LCC, and S-LCA). Thus, it was decided to present the results of the sensitivity analysis of the sustainability index in the article, while the results of the sensitivity analysis in the individual life cycle analyses are presented in detail in the Supplementary Material.

Table IV - 2: Results of sensitivity analyses performed.

Variation	Sustainability index				
	Case study 01 - Brazil	**Case study 02 - China**	**Case study 03 - Spain**	**Case study 04 - Hungary**	**Case study 05 - United States**
(i) Type of injection					
Pressure injection (initial scenario)	0.406	0.518	0.839	0.845	0.903
Gravity injection	0.406	0.518	0.837	0.831	0.902
(ii) Use of other materials in injection wells and monitoring					
Reuse of PVC	0.390	0.515	0.835	0.841	0.897
PVC recycling	0.391	0.513	0.836	0.842	0.897
Polyethylene	0.395	0.517	0.840	0.846	0.903
Polyethylene reuse	0.395	0.517	0.840	0.846	0.903
Recyclable polyethylene	0.396	0.518	0.841	0.847	0.904
Aluminium	0.380	0.502	0.825	0.831	0.884
Aluminum recycling	0.393	0.507	0.830	0.836	0.890
Steel	0.393	0.515	0.839	0.844	0.900
Steel recycling	0.392	0.511	0.837	0.843	0.898
Iron	0.386	0.508	0.831	0.837	0.893
Iron recycling	0.391	0.513	0.833	0.839	0.895

Variation	Sustainability index				
	Case study 01 - Brazil	Case study 02 - China	Case study 03 - Spain	Case study 04 - Hungary	Case study 05 - United States
(iii) On site production of nZVI					
Milling	0.647	0.639	0.840	0.844	0.889
Reduction with sodium borohydride	0.294	0.394	0.838	0.841	0.887
Reduction with hydrogen gas	0.363	0.406	0.840	0.843	0.888
Thermal reduction	0.363	0.406	0.840	0.843	0.888
Chemical vapor deposition	0.606	0.612	0.839	0.842	0.886
Micro-emulsion	0.232	0.283	0.831	0.835	0.801
Ultrasonic waves	0.332	0.378	0.838	0.842	0.883
Eletrochemical	0.662	0.629	0.840	0.843	0.887
Green synthesis	0.615	0.590	0.840	0.843	0.888
(iv) Buy the nZVI from different companies					
Nanoiron s.r.o.(Czech Republic)	0.382	0.499	0.833	0.840	0.882
Toda Kogyo Corp. (Japan)	0.370	0.483	0.834	0.840	0.885
NanoAmor, Amorphous Products (United States)	0.494	0.536	0.832	0.838	0.878
Golder Associates Inc. (United States)	0.494	0.536	0.832	0.838	0.878
Scientific Instruments Dresden GmbH (Germany)	0.496	0.522	0.832	0.837	0.877
Standart deviation	**0.103**	**0.077**	**0.004**	**0.004**	**0.019**

Figure IV - 5: Sensitivity analysis varying the functional unit.



In general, the results of the sustainability index are not very sensitive to the variations considered in this study. The standard deviation was higher in case studies 01

Brazil and 02 China. However, all standard deviations were less than 0.12, which demonstrates that the results are less sensitive.

Variations in the sustainability indexes were observed in case studies 01 Brazil and 02 China in the variations in production at the nZVI sites by different production methods and also in the purchase of nZVI from other companies. These factors can be explained because in these two case studies (01 Brazil and 02 China) the highest amounts of nZVI are used, respectively 21.95 kg and 13.31 kg. Thus, it is perceived that nZVI is one of the factors that influence sustainability when the amount of nZVI used in remediation is high. Therefore, sustainability can vary depending on the scenario considered, whether producing on site or buying from different companies.

Visentin et al. (2022) evaluated the life cycle sustainability of different nZVI production methods and demonstrated that electrochemical, green synthesis, and milling methods are the most sustainable for nZVI production, classified as highly sustainable. Microemulsion methods and ultrasonic waves are the least sustainable. On the other hand, methods that are used in the production of nZVI by different companies resulted in different classifications, such as reduction with hydrogen gas (classified as sustainable), thermal reduction (classified as highly sustainable), and steam deposition (classified as highly sustainable).

Another variation was modification of the functional unit of LCAs. In all the results, the functional unit considered is 1.00 m^3 of remediated soil. For this variation of sensitivity, a functional unit of 1.00 kg of nZVI used in remediation was considered. For this, the inventory data were adjusted to correspond to the functional unit considered.

With the modification of the functional unit, significant variations in the sustainability index of the case studies are perceived. In the functional unit of 1.00 kg of nZVI, case study 02 China resulted in the highest sustainability index (0.67), while the lowest value came from case study 03 Spain (0.58). All cases are classified as sustainable, except for case study 03 Spain, which was classified as neutral. Furthermore, a uniformity of the sustainability index of the case studies is perceived, ranging from 0.58 to 0.67, due to the functional unit being based on the amount of nZVI. The variations in the sustainability index of the case studies demonstrates the difference in the impacts and costs of the different methods of production of nZVI used in the studies, whether they are in on-site production (case studies 02 China and 05 United States) or in the purchase of nZVI (case studies 01 Brazil, 03 Spain, and 04 Hungary).

Compared to the sustainability index data for the functional unit of 1.00 m^3, it is noticed that for case studies 03 Spain, 04 Hungary, and 05 United States, the sustainability index for 1.00 m³ is higher than the value for the functional unit of 1.00 kg of nZVI. This is because these case studies use small amounts of nZVI for the remediation of 1.00 m³. Case studies 01 Brazil and 02 China resulted in higher values for the functional unit of 1.00 kg of nZVI; because the functional unit used is 1.00 m³, the amounts of nZVI used in these case studies are high. When the case studies are unified under the functional unit of 1.00 kg of nZVI, the differences result in the production and purchase data for nZVI in each case study.

It is worth mentioning that for the functional unit of 1.00 kg of nZVI, the amount of remediated soil varies for each case study, depending on the soil characteristics of each site. In case study 01 Brazil, 1.00 kg of nZVI remediates 0.009 m³ of soil, while in case study 02 China, this figure is 0.105 m³. In case study 03 Spain, the amount of remediated soil is 916 m³, while in case study 04 Hungary, 1,075 m³ of soil is remediated. In case study 05 United States, this number is 94.00 m³.

3.5 Factors influencing nZVI sustainability

The sustainability of nZVI is related to various factors: the amount of nZVI used in remediation and production methods, soil types and characteristics, types of contaminants and their concentrations, the injection processes used, and the materials used for remeasurement, such as in injection and monitoring wells.

3.5.1 Quantity of nZVI used and production methods

The main factor that influences the sustainability of contaminated sites remediation with nZVI is the amount of nZVI used in remediation. It is noticed that in case studies 01 Brazil and 02 China, in which the largest amounts of nZVI are used (respectively 21.95 kg and 13.31 kg), the greatest environmental impacts and costs are verified, in addition to lower social factors and, consequently, the lowest sustainability.

In the sensitivity analysis performed using the functional unit of 1.00 kg of nZVI for all case studies, the sustainability index resulted in a smaller variation in the case studies evaluated. Thus, the influence of the amount of nZVI used in remediation with sustainability can be corroborated. The variations observed in the sensitivity analysis result from the type of nZVI used (whether marketed by companies or manufactured on site) and the synthesis process of nZVI. As presented by Visentin et al. (2022), there are nine production methods that are used both in laboratory production at the remediation site and in industrial production of nZVI for companies that sell it. Among these methods, electrochemical methods, green synthesis, milling, vapor deposition, and hot reduction are the most sustainable. The methods used in the production of nZVI by companies that market it are reduction with hydrogen gas, thermal reduction, chemical vapor deposition, and milling, which result in sustainability indexes exceeding 0.78.

The synthesis of nZVI at the remediation site can contribute to improving the sustainability of the process. Because transport impacts are minimized, however, costs may be higher depending on the synthesis methods used. Case studies 02 China and 05 United States carried out the production of nZVI at remediation sites using the chemical reduction method with sodium borohydride. For case study 02 China, the sensitivity analysis considering the functional unit of 1.00 kg of nZVI resulted in the highest sustainability index.

Thus, the sustainability of the use of nZVI in remediation is directly related to the amount of nZVI to be used in the process, which depends on the type of soil, saturation level, and contaminant. Bench tests are typically used to define the concentration of nZVI to be used in remediation. The nZVI used in remediation and its synthesis method also contribute to the sustainability of the process.

3.5.2 Soil saturation level

Another factor that was verified that has a direct influence on the sustainability of the use of nZVI in remediation is the level of soil saturation. In this article, case studies with different soil types were selected: saturated and unsaturated, and composed of finer or coarser grains. Varying soil types contribute to differences in the concentration and amount of nZVI used in remediation.

The injection of nZVI is a common method in the remediation of saturated soils, unlike the remediation of unsaturated soils as in case studies 01 Brazil and 02 China. Thus, there is not the same proportion of pilot-scale studies or field applications that use nZVI in the remediation of unsaturated soils compared to studies for saturated soils.

Based on the inventory data presented previously, the amount of nZVI used in the remediation of unsaturated soils is much higher compared to the amount used in saturated soils. The amounts of nZVI used in case studies 01 Brazil and 02 China are 21.95 kg and 13.31 kg, respectively. There is still no specific scientific evidence that can clarify this difference in the amount of nZVI used in the remediation of saturated and unsaturated soils. This analysis was performed based on the data verified in the selected case studies.

For example, in case study 01 Brazil, for soil contaminated with hexavalent chromium and PCE, the concentration of nZVI used was 40 g/kg. However, in case study 05 United States, contamination by various organic compounds, including PCE, resulted in a maximum concentration of nZVI of 10 g/L for remediation. A relationship between soil and water density demonstrates the difference in the amounts of nZVI used in the two case studies since the soil density of case study 01 Brazil is approximately 1.66 times greater than the water density.

The retention mechanisms in the unsaturated zone are more complex than in the saturated zone, mainly due to the presence of an air phase in the system (Bradford and Torkzaban 2008; Soares et al. 2018; Reginatto et al. 2020). In addition, knowledge of the mobility of nanoparticles in porous media and the processes that affect their movement is limited, mainly for unsaturated soil, due to the complex nature of the interactions between nZVI and the soil matrix (Tiede et al. 2009; Tourinho et al. 2012; Hosseini and Tosco 2013; Saberinasr et al. 2016; Soares et al. 2018).

Using sandy soil, Soares et al. (2018) evaluated the transport of nZVI in saturated and unsaturated soils in order to identify which type of injection sequence would be most appropriate for each soil. The authors concluded that in saturated soils, the transport of nZVI is lower along the soil column than in unsaturated soil, in which the flow paths are all clear and allow the free movement of nZVI. Thus, it is perceived that in saturated soils the movement of nZVI is more difficult but allows for more homogeneous distribution along the soil column.

Rahmatpour et al. (2018) evaluated the dispersion of silver nanoparticles in intact columns of calcareous soils. The authors verified that the dispersion of silver nanoparticles in unsaturated soils was higher than in saturated soils. This explains why, in unsaturated soils, a greater amount of nZVI is required for remediation due to a higher percolating capacity than in saturated soils. However, there are still many gaps to be filled to explain the behavior of nZVI in saturated and unsaturated soils, in addition to a possible relationship between saturation and the amount of nZVI used in remediation.

In unsaturated soils, a greater amount of nZVI may be required for remediation compared to saturated soils. Thus, in studies in which higher amounts of nZVI are used, environmental impacts and costs tend to be higher and sustainability tends to be lower compared to saturated soils, which require lower amounts of nZVI for remediation (see case studies 03 Spain, 04 Hungary, and 05 United States).

3.5.3 Soil particle size

Another factor considered in these case studies is the different soil types, which may influence the amount of nZVI used in remediation. Nanoparticles in porous media tend to be retained, gradually accumulated, or transported with flow (Ling et al. 2021). The main mechanisms that influence the behavior of nanoparticles in soils are ripening, desorption, deformation, blockage, aggregation, and adsorption (Saberinasr et al. 2018; Reginatto et al. 2020; Ling et al. 2021).

Fine soils such as clay and silt significantly affect the behavior of the transport of nanoparticles through interception, adsorption, blockade, and preferential flow (Mitropoulou et al. 2013; Sun et al. 2015; Lv et al. 2016; Dong et al. 2020; Johnson et al. 2020). With smaller soil grain sizes, the penetration rate of nZVI in the sand column decreases (Mattison et al. 2011). Smaller particle sizes increase the specific surface area, further retaining nanoparticles through physical-chemical adsorption (Braun et al. 2015). In addition, in soils with smaller particles, there may also be agglomeration and retention of nZVI, with the least mobile and concentrated nanoparticles near the injection point or in a restricted area of the soil (Ling et al. 2021).

Soares et al. (2018) evaluated the influence of particle size on nZVI mobility in sandy soil. The authors concluded that using the same injection sequence and water saturation level, in soils with smaller particle sizes, the nZVI is retained more, making it more difficult to transport along the column. This was also observed by Sun et al. (2015), who studied the transport of other nanoparticles and graphene oxide in columns of sand. Kasel et al. (2013) and Liang et al. (2013) explained that retention/filtration can be attributed to increased nZVI mass transfer from the aqueous phase to the surface of the soil particle as the particle size decreases.

Regarding the amount of nZVI in different soil types, it was identified based on the case studies that there is a relationship between these factors. Case study 01 Brazil is composed of an unsaturated clay soil (tropical, residual structured, with kaolinite as the predominant clay mineral, which confers the characteristic of greater permeability compared with fine sand); however, with high negative surface charges, it promotes greater reactivity with nanoparticles. As time goes by, a larger number of particles will adhere to the soil grains, reducing the size of the soil void. It starts to function more as a filter, retaining more nZVI that is passing through and modifying the electrochemical balance (Reddy 2010; Reginatto et al. 2020). This results in a greater amount of nZVI being used in the remediation of 1.00 m^3 of soil. Case study 02 China corresponds to unsaturated soil, composed mainly of sand grains, which confers a greater permeability to the soil and results in a smaller amount of nZVI needed for remediation. It should be noted that in both case studies the contaminant used was hexavalent chromium, and the concentration of nZVI was different by a magnitude of 3,600 times (40 g/kg and 11 mg/kg).

3.5.4 Soil permeability

Permeability is a characteristic of soil that can influence the sustainability of using nZVI in remediation. Depending on soil permeability, nZVI transport can be facilitated or prevented. In addition, permeability also influences the injection pressure of nanoparticles, which are difficult to inject by gravity in poorly permeable soils.

In soils with high permeability or with zones of high permeability (coarse sand with a porosity of 0.4), nZVI tends to be transported by these sites (Velimirovic et al. 2020). However, in very permeable, porous media, the high speed of groundwater reduces the efficiency of in situ remediation, reducing the time of contact with contaminants (Aranda et al. 2020).

The transport of nZVI in soils of low permeability and fine granulometry is more difficult compared to soils of high permeability. When the size of nanoparticles is greater than or equal to the size of the soil grains, nanomaterials are likely to become trapped in small pore throats, blocking or tensioning and resulting in a decrease in permeability and a high deposition of nanoparticles (Hosseini and Tosco 2013; El-Amin et al. 2015; Salama et al. 2015; Chequer et al. 2018; Ling et al. 2020).

In soils with high permeability, gravity injection may be an alternative because the transport of nanoparticles is facilitated. In gravity injection, some changes in environmental, economic, and social impacts can be verified, as detailed in the sequence items 3.5.6. On the other hand, in soils with low permeability and porosity, gravity injection can be hindered and result in a longer remediation time because the transport of nanoparticles through the pore medium of the soil is more difficult.

In addition, the pressure at the nanoparticle entry point may increase over time due to low permeability, causing a large angle of media anisotropy and preventing the subsequent transport of nanoparticles (Chen et al. 2016). Given that nanoparticles tend to transport preferentially and then remain in areas of high permeability (e.g., coarse gravel sand), the available pore space and permeability can be decreased.

3.5.5 Type of contaminant

The type of contaminant verified at the site to be remedied can also contribute to the sustainability of nZVI in remediation. Depending on the type of contaminant, the required concentration of nZVI may be higher or lower. There is no nZVI concentration pattern for each type of contaminant. The concentration is determined on the basis of bench tests that consider the soil characteristics of the site, the concentration of the contaminant, and different concentrations of nZVI to determine the appropriate concentration.

In the saturated soils of case studies 03 Spain, 04 Hungary, and 05 United States with organic and inorganic contaminants, the concentration of nZVI was the same at 10g/L. In case studies 01 Brazil and 02 China, which have unsaturated soils contaminated with hexavalent chromium, there is a small variation in the concentration of nZVI used. In case study 01 Brazil, the concentration of nZVI used was 12.5 mg/kg, while in case study 02 China, the concentration was 11 mg/kg. Thus, considering only the cases in this study, the greatest difference in the concentration of nZVI is due to the level of soil saturation and not the type of contaminant.

In the case of hexavalent chromium, for example, nZVI concentrations may vary depending on the type of nZVI used, the type of soil, and also the concentration of chromium in the soil to be remedied. In case studies 01 Brazil and 02 China, the concentration of nZVI was 40 g/kg and 11 mg/kg, respectively, while chromium contamination concentration was 100 mg/kg and 800 mg/kg, respectively. Other concentrations were used, for example, by Pei et al. (2020) at 50 g/kg (Cr (VI) concentration of 198.20 mg/kg) and Liu et al. (2020) at 5 g/L (Cr (VI) concentration of 15.68 mg/L).

In organic contaminants, variations are also perceived. In case studies 04 Hungary and 05 United States, the concentration used was 10 g/L for organochlorinated compounds (see contamination concentrations in Table 1). Other concentrations were used for organochlorinated compounds, for example, by Kocur et al. (2016) at 1 g/L, Gavaskar et al. (2005) and Lacina et al. (2015) at 2 g/L, Elliott and Zhang (2001) at 1.5 g/L and 0.75 g/L, Köber et al. (2014) and Bitsch et al. (2017) at 10 g/L, and Jordan et al. (2013) at 21.5 g/L.

3.5.6 Injection process

The nZVI injection process in remediation does not influence the sustainability of nZVI. The sensitivity analysis performed considering injection under pressure or gravity injection did not result in differences in the sustainability indexes of the case studies.

In the individual analyses of the life cycle, some differences in environmental impacts are perceived (in the Supplementary Material, the results of the sensitivity analysis in the LCAs are presented), being in most cases higher in injection under pressure than in gravity injection due to lower energy consumption. However, gravity injection can increase injection time and consequently the work of operators and machinery, which can also contribute to increased costs.

3.5.7 Materials used in remediation wells

Like the injection process, the materials used in remediation, in this case the materials used in the injection and monitoring wells, do not influence the sustainability of nZVI in remediation.

However, in the individual sensitivity analyses of LCA (LCA, LCC, and S-LCA) (see Supplementary Material), there is a difference in environmental impacts, which are greater when considering injection tubes and monitoring of steel, aluminum, or iron (increase of about 11% in environmental impacts). However, recycling or reusing these pipes reduces an average of 5% of the environmental impacts.

3.5.8 Location of the remedied site

Another factor that can influence the sustainability of nZVI in remediation is the location of the area to be remedied. This factor can contribute to the type of soil and consequently to the amount of nZVI necessary for remediation, as well as in relation to social aspects, remediation costs, environmental impacts, and the feasibility of using nanoremediation.

As verified in the results of the S-LCA, developing countries have lower social life cycle scores compared to developed countries. In the case studies in this article, the social life cycle scores are lower in case studies 01 Brazil and 02 China than in the other case studies (03 Spain, 04 Hungary, and 05 United States). Visentin et al. (2021c) demonstrated that social life cycle scores are highly dependent on the social situation of a given country; in this study, for example, the authors present the differences in the index considering the locations of Brazil and Switzerland. Developed countries with better social indicators result in higher social life cycle scores and consequently better sustainability indexes (Visentin et al. 2021a, 2021c).

Costs can also be influenced, for example, by the costs of raw materials, energy, and labor. In the cases presented in this study, there are labor costs for skilled labor, ranging from \$5.51/h in China to \$36.64/h in the United States. In addition, material transportation costs may also be influenced depending on location. In the case studies in which nZVI is purchased from different companies (case studies 01 Brazil, 03 Spain, and 04 Hungary), it is noticed that the value of transport varies from 22% to 37% of the total costs of the life cycle.

In environmental impacts, location contributes to impacts related to energy consumption, which, depending on the country and its energy matrix, can result in greater or lower environmental impacts. Visentin et al. (2019b) found that in countries with energy matrixes of non-renewable sources, environmental impacts are greater than in countries with energy matrixes based on renewable sources. For example, in the case presented in Visentin et al. (2019b) for an nZVI production method with high energy consumption (above 90 kWh), the environmental impacts of the United States are more than 70% higher than Brazil's environmental impacts.

Visentin et al. (2021a) evaluated the influence of location on the sustainability index of nZVI production methods, considering the United States, Europe, Japan, and Brazil. In this analysis, it was possible to verify that the most sustainable scenario was in Europe for all the methods evaluated. In the methods with higher energy consumption, the United States produced less sustainability. For methods with lower energy consumption, Brazil resulted in lower sustainability due to the lower social index.

Another factor that stands out in localization is in relation to the feasibility of using nanotechnology. To date, there have been relatively few commercial deployments of nanoremediation. Bardos et al. (2018) cite 100 examples of field-scale applications of nZVI on a pilot scale and real scale. This fact is explained by uncertainties, relatively high material costs, and the perception that the benefits generally do not outweigh the risks in the context of sustainable risk management (Bone et al. 2020).

In Brazil, for example, the use of nanomaterials in remediation is still in the laboratory phase. This is due to numerous factors; for example, nanoremediation is not a widely disseminated and available technology in the country. Thus, the use of nanoremediation is restricted on a scientific laboratory scale and is not used by companies that commercialize remediation techniques. Usually, companies that commercialize remediation in Brazil recommend the use of available technologies from their own domains instead of expanding to other techniques (e.g., air sparging, bioremediation, pump and treat, free phase recovery, multiphase extraction, and soil/residue removal). In addition, the transport costs of commercial nZVI may also make it difficult to apply the technology in Brazil.

Still, in many countries, the concern with sustainability in remediation is not yet widespread; knowledge still concentrates significantly in academia and is not exploited by the government and decision makers. The choice of remediation process is based on costs and ease of use, not on sustainability. This is demonstrated by the differences between developed and developing countries. Thus, the public authorities and remediation industries of relevant countries needs to show greater interest and take initiatives for a more efficient management of contaminated sites (Braun et al. 2020).

4 Conclusion

This article evaluates the sustainability of the life cycle of nZVI used in remediation through five case studies of remediation of contaminated sites in different locations in the world with different types of contaminants and soils.

Case study 01 Brazil resulted in the greatest environmental impacts and case study 04 Hungary in the smallest. Case study 02 China resulted in the highest life cycle costs and case study 04 Hungary in the smallest. Case study 01 Brazil resulted in the lowest social life cycle score, while case study 05 United States had the highest. For LCSA, case study 05 United States was the most sustainable, while case study 01 Brazil resulted in the lowest sustainability.

Different sensitivity analyses were performed in order to verify the influence of several factors on the sustainability indexes. In all analyses, the results were sensitive only to changes in the functional unit of LCA.

Finally, based on the results of the ASCV of the case studies it was possible to determine some factors that directly contributed to the sustainability of using nZVI in remediation: amount of nZVI used in remediation, saturation level, soil particle size, permeability, type of contaminant, and location of remediation. The injection process and the material used in the injection wells did not contribute significantly to the sustainability of the use of nZVI in remediation.

This work filled an important scientific gap, presenting in detail the sustainability of the use of nZVI in the remediation of contaminated sites. The selection of different case studies contributed to an important conclusion regarding the factors that influence the sustainability of the use of nZVI in remediation. Future research should verify whether there are practical relationships between the soil saturation level with the amount of nZVI used in remediation. And also, future research can compare nanoremediation with nZVI with other remediation technologies, to verify that nZVI is sustainable compared to traditional remediation techniques.

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Supplemental Material

Case studies description

- **Case Study 01, Brazil (Vanzetto & Thomé, 2022).**

Case study 01 corresponds to the use of nZVI on a field scale in the remediation of contaminated soils in southern Brazil (Vanzetto; Thomé, 2022). In this study, the remediation took place in unsaturated soil. The site was contaminated with hexavalent chromium Cr(VI)and pentachlorophenol (PCP). The Cr (VI) concentration is 100 mg/kg, and the intervention value in Brazil is 0.4 mg/kg, while the PCP concentration is 100 mg/kg, with an intervention value of 0.16 mg/kg.

The volume of remedied soil was estimated at 0.2 m^3. The site's soil is clayey, composed of 72% clay, 15% silt, and 13% sand. It is a tropical soil, residual structured, with kaolinite being the predominant clay mineral, which confers the characteristic of greater permeability in relation to unstructured clayey soils. The hydraulic conductivity of the soil is 1.39x10-3 cm/s and the moisture is 34%.

The remediation process was carried out by injection under pressure of the nZVI suspension. The injection was performed by a rod with 12 holes of 1.0 mm in diameter, arranged in 30-degree radii, with an injection pressure of 90 psi lasting 6 minutes, with an injection rate of 2 L/min. A total of 4.39 kg of nZVI was injected. The nZVI used was Nanofer Star from Nano Iron s.r.o. located in the Czech Republic. The activation of the nanoparticle occurred according to the manufacturer's instructions, at a concentration of 40 g/kg. The remediation efficiency was greater than 90%. Data were collected at 48 sampling points and monitored during a 90-day period.

- **Case Study 02, China (Zhang et al. 2019)**

Case study 02 corresponds to the study by Zhang et al. (2019) referring to in situ remediation on a laboratory scale with Carboxymethyl cellulose (CMC)-stabilized nanoscale zero-valent iron (CMC-nZVI) in a soil contaminated with hexavalent chromium in Guangzhou, China. The soil used in the study is composed of 59% sand; 22.5% silt and 18.5% clay, with density of 1.21 KN/m^3 and hydraulic conductivity of $5.36x10^{-4}$ cm/s (Liu et al. 2020). The soil was contaminated with Cr (VI) at a concentration of 800 mg/L Cr, and the intervention value in China is 5 mg/kg (Sun et al. 2019).

The nZVI-CMC used in the study was synthesized on site using the chemical reduction method with sodium borohydride. The study was carried out with 1.00 kg of soil contaminated with Cr (VI), and the optimum concentration of nZVI-CMC was 11 mg/kg of contaminated soil.

In the study, remediation occurred by mixing nZVI-CMC with contaminated soil, however, in real field situations, the injection process is usually used. Thus, for life cycle analyses, the injection data of the study by Song et al were used as the basis. (2020), because it is applied in a soil of China with characteristics similar to that of the study by Zhang et al. (2019). Thus, the injection under pressure was considered with a rate of 0.05 L/min. The resulting remediation efficiency was 95% (Zhang et al. 2019). The monitoring was carried out in twenty points, in 8 days of monitoring during the period of 120 days.

- **Case Study 03, Spain (Otaegi & Cagigal, 2017)**

Case study 03 corresponded to pilot-scale use in remediation with nZVI in a nitrastur contaminated area in Asturias, Spain (Otaegi and Cagigal, 2017). This study was undertaken as part of the NanoRem Project (Taking Nanotechnological Remediation Processes from Lab Scale to End User Applications for the Restoration of a Clean Environment), which was funded through the European Union Seventh Framework Programme.

The study site is a 20-hectare brownfield, which was used between 1950 and 1998 for the production of nitrogen-based products as fertilizers. The site is contaminated with heavy metals, the main being arsenic in groundwater, in the forms of As (V) and As (III). The maximum arsenic concentration detected in groundwater was 5527 μg/l, while the Dutch intervention value is 60 μg/l.

The volume of contaminated soil was estimated at up to 228,904 m^3. The soil of the remediation site is composed of sandy gravels with boulders. Hydraulic conductivity of 5.7×10^{-4} cm/s.

Site remediation occurred in February 2016, and was performed by injection under nZVI pressure. The injection occurred in three injection points in a triangular configuration, low pressure (< 5bar) and a flow rate of approximately 0.6 - 1m^3/hour, (more information can be verified in Otaegi and Cagigal, 2017). A total of 250 kg of nZVI was injected into the pilot area. The nZVI used was nanofer star from NanoIron located in the Czech Republic. Before the injection of nZVI, activation was made with water and agitation according to the manufacturer's guidance, at a concentration of 10 g/L. Remediation efficiency was above 90%. Monitoring was performed through eight monitoring wells and was performed in 28 days, from the day of injection to six months after remediation.

- **Case Study 04, Hungary (Laszlo & Szabo, 2017)**

Case study 04 is also part of the NanoRem project to remedy groundwater contaminated with chlorinated hydrocarbons in a contaminated area in Balassagyarmat, Hungary (Laszlo and Szabo, 2017). The study site is an industrial brownfield, which was used between 1970-1994, for the production of electrical components for the industry.

Site contamination was composed of hydrocarbons chlorinated mainly with CHCs, such as perchloroethylene (PCE), trichloroethylene (TCE) and dichloroethylene (DCE). The contaminated plume is estimated to contain 15 kg of HCP (95% PCE). The highest concentrations of contaminants indicated were 15-20,000 µg/L.

The volume of contaminated groundwater is estimated at about 190,000 m^3. The soil of the remediation site is composed of layers of sandy gravel, silt clay and holocene sand, and most of the plume was verified in the sandy gravel layer. Hydraulic conductivity of $7.6x10^{-2}$ cm/s.

Site remediation occurred in September 2015, and was performed by injection under pressure from nZVI. The nZVI used for remediation was provided by ScIDre GmbH from Dresden, Germany. Before remediation the suspension was prepared, mixing the nZVI with oxygen-free water using tanks, at a concentration of 10 g/L. The suspension was pumped from the tanks to the injection well used a hydraulic pump. The injection occurred under pressure of 0.5 to 5 bar in three injection wells, at a rate of 20 – 30 L/min. A whole, 176.8 kg of nZVI were injected. The remediation efficiency was above 60%. Monitoring was carried out in 14 wells, in 8 days of monitoring during the period of -5 to 360 days.

- **Case Study 05, United States (He et al. 2010)**

Case study 05 corresponds to the study by He et al. (2010) who conducted a pilot test at a former factory located in the southern U.S. Site contamination is characterized by organochloroethene compounds such as PCE, TCE, cis-dichloroethene (cis-DCE), trans-dichloroethene (trans-DCE), and vinyl chloride (VC), along with PCB1242 have been detected in the groundwater. The concentration of site contamination was PCE = 1.20 – 12.0 mg/L, TCE = 1.6–23.8 mg/L, cis-DCE = 8.5–20 mg/L, VC = 1.1–2.2 mg/L and PCB1242 = 6.9– 97.4 µg/L.

The volume of soil to be remedied was estimated at 64.10 m³. The soil of the site is composed of a mixture of silt, fragments of siliceous limestone gravel and a small fraction of clay. The layer of sand and gravel makes this area relatively permeable. The hydraulic conductivity of the soil is $1.98x10^{-3}$ cm/s.

The remediation of the site took place in January and February 2007. And the remediation process was performed by injecting nZVI in two stages. The first injection occurred by gravity and the second under pressure. The first injection was performed using a peristaltic pump to transport the nZVI suspension from the tank to the injection well, the pump did not exert injection pressure. The injection rate was 2.54 L/min, and lasted 3.7 hours. The second injection occurred under pressure, and in this case the pump exerted injection pressure, which was less than 0.35 bar. The injection rate was 5 L/min and lasted 1.8 hours.

The nZVI used in remediation was produced on site using the chemical reduction method with sodium borohydride. The injection of the nanoparticles was performed through a suspension, which was made before each injection. In the first injection, 114 g of nZVI was used at a concentration of 0.2 g/L, while in the second injection they were 569 g at a concentration of 10 g/L. The remediation efficiency verified was above 90%.

The monitoring was carried out in three wells, in 20 days of monitoring during the period from 0 to 600 days.

Inventory

Table IV - 3 presents the environmental and economic inventory data of the five-case study of nZVI remediation. All data are based on the functional unit of life of 1.00 m³ of soil remediated. Table IV - 4 details the categories of impact and social indicators. Table IV - 3: Environmental and economic inventory of case studies.

Case studie	Stages	Inputs and outputs	Amount	Costs
01 – Brazil Vanzetto & Thomé (2022)	nZVI production	nZVI (NANOFER STAR)	21.95 kg	6.05 $/kg
	Transport	Airplane	244.75 tkm	1.57 $/tkm
		Truck	6.33 tkm	2.58 $/km
	Site preparation	PVC pipes	3 m	20.34 $/m
		Excavation	1 h	100 $/h
		Transport	60 km	0.53 $/km
		Solid waste	22 kg	0.07 $/kg
	Activation	Deionized water	$6.5x10^{-2}$ m³	0.04 $/m³
		Energy	0.134 kWh	0.16 $/kWh
		Solid waste	0.5 kg	0.07 $/kg
	Injection	Energy	0.96 kWh	0.16 $/kWh
	Monitoring	Energy	0.6 kWh	0.16 $/kWh
		Wastewater	8 $x10^{-3}$ m³	0.15 $/m³
		Solid waste	0.2 kg	0.07 $/kg
	Labor costs		5 h	10.70 $/h
02 – China Zhang et al. (2018)	nZVI production	On-site production, reduction with sodium borohydride method	13.31 kg	296.36 $/kg
	Site preparation	PVC pipes	3 m	20.34 $/m
		Excavation	1 h	100 $/h
		Transport	60 km	0.53 $/km
		Solid waste	16 kg	0.07 $/kg
	Activation	Deionized water	0.039 m³	0.04 $/m³
		Energy	0.134 kWh	0.01 $/kWh
	Injection	Energy	0.965 kWh	0.01 $/kWh
	Monitoring	Energy	0.525 kWh	0.01 $/kWh
		Wastewater	1.5 $x10^{-3}$ m³	0.15 $/m³
		Solid waste	0.2 kg	0.07 $/kg
	Labor costs		5 h	5.51 $/h
03 – Spain Otaegi & Cagigal (2017)	nZVI production	nZVI (NANOFER STAR)	1.09 g	6.05 $/kg
	Transport	Airplane	$2.08x10^{-3}$ tkm	74216.35 $/tkm
	Site preparation	PVC pipes	3 m	20.34 $/m
		Excavation	1 h	100 $/h
		Transport	60 km	0.53 $/km
		Solid waste	22.51 kg	0.07 $/kg
	Activation	Deionized water	$1.09x10^{-4}$ m³	0.04 $/m³
		Energy	3.168 kWh	0.12 $/kWh
		Solid waste	$1x10^{-2}$ kg	0.07 $/kg
	Injection	Energy	7.63 kWh	0.12 $/kWh
	Monitoring	Energy	1.05 kWh	0.12 $/kWh
		Wastewater	2.8 $x10^{-3}$ m³	0.15 $/m³
		Solid waste	0.1 kg	0.07 $/kg

	Labor costs		14 h	22.80 $/h
04 – Hungary Laszlo & Szabo (2017)	nZVI production	nZVI (Carbo Iron SciDre)	0.93 g	18218.9 $/kg
	Transport	Airplane	$4.9x10^{-3}$ tkm	29636.73 $/tkm
	Site preparation	PVC pipes	3 m	20.34 $/m
		Excavation	1 h	100 $/h
		Transport	60 km	0.53 $/km
		Solid waste	22.6 kg	0.07 $/kg
	Activation	Deionized water	$6.5x10^{-5}$ m³	0.04 $/m³
		Energy	0.216 kWh	0.15 $/kWh
		Solid waste	$1x10^{-2}$ kg	0.07 $/kg
	Injection	Energy	0.52 kWh	0.15 $/kWh
	Monitoring	Energy	0.3 kWh	0.15 $/kWh
		Wastewater	8.9 $x10^{-3}$ m³	0.15 $/m³
		Solid waste	0.1 kg	0.07 $/kg
	Labor costs		5 h	9.90 $/h
04 – United States He et al. (2010)	nZVI production	On-site production, reduction with sodium borohydride method	10.62 g	874.9 $/kg
	Site preparation	PVC pipes	3 m	20.34 $/m
		Excavation	1 h	100 $/h
		Transport	60 km	0.53 $/km
		Solid waste	19.87 kg	0.07 $/kg
	Activation	Deionized water	$8.8x10^{-3}$ m³	0.04 $/m³
		Energy	0.8 kWh	0.06 $/kWh
	Injection	Energy	3.35 kWh	0.06 $/kWh
	Monitoring	Energy	0.56 kWh	0.06 $/kWh
		Wastewater	$1.5x10^{-3}$ m³	0.15 $/m³
		Solid waste	0.1 kg	0.07 $/kg
	Labor costs		10 h	36.64 $/h

Table IV - 4: Categories of impacts, indicators and data source of S-LCA indicators.

***Stakeholders* categories**	**Impacts categories**	**Indicators**	**Source**
Workers	Freedom of negotiation and collective association	Cooperation in work-employer relations	WEF (2020)
		Hiring and firing practices	
	Child labor	Child labor	WHO and UNICEF (2020)
		Number of children out of school	
	Fair wage	Minimum wage (U$/month)	ILO (2020)
		Flexibility in determining wages	WEF (2020)
		Remuneration and productivity	
	Working hours	Average working hours	OCDE (2021)
		Women's participation in the workforce	WEF (2021)

	Equal opportunity/discrimination	Equal pay for similar work	
	Health and safety	Occurrence of lethal occupational accidents per year	ILO (2020)
		Occurrence of non-lethal occupational accidents per year	
		Workers' exposure to chemicals and contaminants	Regarding the operation of each case study.
		Generation of hazardous waste and effluents	
		Health risks during the production process (emission of hazardous gases during production)	
Local Community	Safe and healthy living conditions	Carbon intensity	WEF (2020a)
		Contribution to global warming	Regarding the operation of each case study, based on LCA results.
		Quality of ecosystems	
		Exposure to contaminants (emission of gases that affect human health)	
		Resource usage	
	Access to material resources	Population with access to improved drinking water	WEF (2020)
		Population with access to improved sanitation	WHO and UNICEF (2020)
		Quality of electricity supply	
Consumer	Health and safety	Exposure to chemicals and contaminants	Regarding the operation of each case study, and information made available on the website of each company that markets the nZVI
		Health risks during the application process	
		Existence of health and safety measures for product application	
	Product application	Extra working time for the consumer to apply the product	
		Average prices for application	
		Level of complexity for calculating dosages	
		Main consumer concerns about the product.	
	Return mechanisms	Contact with the production company responsible for the product	
		Distance from responsible company to consumer	
	Transparency	Availability of information on social and environmental performance	
	End-of-life responsibility	Need for control with the end of the life of the product	
Society	Market and work	Country unemployment rate	WEF (2020)
		Labor market efficiency	
	Contribution to economic development	Extension of marketing	
		Sophistication of the production process	
		Collaboration between university and industry	
	Governance	Efficiency of government spending	
		Transparency in government policy making	
		Total tax rate	
Value chain	Fair competition	Intensity of local competition	
	Promotion of social responsibility	Ability to promote social responsibility	

	Relations with suppliers	Relationship with suppliers	

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3. CAPÍTULO V (artigo de resultados - não submetido): Environmental, economic and social viability in the use of nano scale zero valent iron for soil and groundwater remediation: An analysis of sustainability from the Brazilian perspective

Abstract: The use of nanomaterials in remediation has emerged as an innovative and promising technology. However, in practice there are still many difficulties to enable the use of nanomaterials in remediation. The nano scale zero valent iron (nZVI) is the main nanomaterial studied and used in remediation. Thus, the objective of this work is to verify the viability, in relation to sustainable terms, of the use of nanoremediation with nZVI in contaminated areas, considering a perspective of Brazil. The study was carried out considering an area contaminated with chromium in two remediation scenarios, scenario I unsaturated soil and scenario II saturated soil. Different remediation techniques were selected for the remediation of each scenario. Viability was analyzed considering life cycle analysis tools, thus, four life cycle analyses were performed, encompassing the environmental, economic, social impacts and sustainability of the life cycle of each remediation technique. The functional unit of the life cycle analyses considered was 10 m^3 of soil and groundwater remediated. The results indicated that nanoremediation with commercial nZVI is not feasible for use in unsaturated soils in Brazil. This technique resulted in the greatest environmental impacts and costs, in addition to lower social index and lower sustainability. Nanoremediation using nZVI produced on site by the green synthesis method makes the use in remediation feasible. On the other hand, in the scenario II of saturated soils, nanoremediation with commercial nZVI is feasible and sustainable for use in Brazil. In general, this study contributes significantly to the state of the art on the impacts and sustainability of nanoremediation, presenting data and analyses not yet scientifically explored, especially in the context of Brazil. The viability of nanoremediation can be directly related to the level of soil saturation and also the amount of nanomaterial used in remediation.

Key-words: Life cycle assessment; soil saturation, nanoremediation; remediation techniques; sustainable remediation.

1. Introduction

Contamination of soils and groundwater in industrial and urban sites is a global problem that results in environment and humans' risks (Braun et al. 2020a; Alazaiza et al. 2021). Numerous studies have been published over the years evaluating the different remediation techniques, their efficiency, applicability, optimization in soil remediation and groundwater polluted by various types of contaminants (Liu et al. 2018).

Numerous techniques can be used in the remediation of soils and groundwater. There are techniques that can be applied in in situ remediation, as well as ex situ; using electricity, heat, and various materials to remove contaminants from soil and groundwater (Hamadani et al. 2020; Hussain et al. 2022). Among the remediation techniques, in recent years there is a highlight in nanoremediation, which is based on the use of nanomaterials in remediation (Thomé et al. 2015; Garnie et al. 2021).

Nanoremediation emerged in the 1990s in the United States as a promising remediation technology. Nanoremediation is an effective, fast and efficient technology for the remediation of various types of pollutants, such as oil and heavy metals, and was therefore considered as a great promise of success in the remediation of soils and groundwater in the world (Alazaiza et al. 2021). The main advantage of nanoremediation is its greater reactivity compared to materials with the same macro-scale composition. Nanomaterials have smaller particle size and larger specific surface area, which results in a greater number of atoms on surfaces allowing a significantly greater number of reactions with contaminants (Thomé et al. 2015; Kumar et al. 2021). The main nanomaterials studied are the nano scale zero valente iron (nZVI), carbon nanotubes; metallic and magnetic nanoparticles (Garnie et al. 2021).

In 2007, a European report predicted that in 2010 the world market for environmental nanotechnologies would be around US$ 6 billion (Rickerby and Morrison, 2007; Bards et al. 2018). However, it is noticed that nanoremediation is a much-studied technique, but little used in the remediation of practical cases in the world (Bone et al. 2020). Bards et al. (2018) cite 100 examples of nZVI applications on a pilot and field scale. The uncertainties associated with nanoremediation caused the technique not to reach the estimated growth, and the adoption of the technique has been relatively slow compared to other technologies (Bardos et al. 2018). It is not yet clear, for example, the environmental risks of nanomaterials in the environment over the years and also the toxicological effects on soil microorganisms and humans with exposure to nanomaterials (Vanzetto and Thomé, 2019; Alazaiza et al. 2021).

Thus, some projects in the world have been carried out in order to expand knowledge about the use of nanoremediation, such as in the United States and Europe. In the United States, selected full-scale, field and pilot nanotechnology applications have been performed and the summary of information can be verified in the Project Profiles Database, which is a database developed by the U.S. Environmental Protection Agency. In Europe, the Project NanoRem, (Taking Nanotechnological Remediation Processes from Lab Scale to End User Applications for the Restoration of a Clean Environment) is a research project, funded through the European Commission FP7, focuses on facilitating practical, safe, economic and exploitable nanotechnology for in situ remediation (Bardos et al. 2018).

In Brazil, few states have a record of contaminated areas (Braun et al. 2020b). The State of São Paulo, which leads the contaminated area management market in Brazil, registered in 2020 more than 1,463 areas in the process of remediation (CETESB, 2021). The main source of contamination identified is the fuel stations, followed by industries, which account for 90% of polluting activities. The main contaminants verified are automotive fuels, aromatic solvents, polycyclic aromatic hydrocarbons and metals. While the main remediation techniques used in Brazil are multiphase extraction, pumping and treatment, free phase recovery, monitored natural attenuation, soil/residue removal, chemical oxidation and vapor extraction. These techniques were used in more than 89% of the remediated areas. In the country, nanoremediation was not used in any remediation process in the State of São Paulo. However, laboratory-scale studies on the technique are representative in the country (Cecchin et al. 2018; Reginatto et al. 2020a, 2020b; Thomé et al. 2020; Cecchin et al. 2021; Basegio et al. 2022; Oca-vásquez et al. 2022).

One of the possible contributions to the non-use of nanoremediation in the world may be related to the way of choosing the remediation technique to be used. Over the years, numerous changes in the management of contaminated areas have been observed. In 1970, decision-makers' concerns were based on the costs of remediation processes, moving in 1980 to an approach based on the availability and feasibility of technologies (Pollard et al. 2004) and 1990 for the risk approach. In the 2000s, concern about environmental, social and economic impacts began to be used in the decision-making process, through the application of the concepts of sustainable remediation (Rizzo et al. 2016). In many countries sustainable remediation has been growing, with studies and public motivation (Braun et al. 2020b). However, in developing countries such as Brazil, in practice it is perceived that the definition of the remediation technique is still related to the availability of technology and the costs of remediation, and for this reason there is also no initiative for the application of nanoremediation in the country.

Chapter IV demonstrated through a life cycle sustainability analysis the environmental, economic and social impact of the use of nZVI in the remediation of contaminated areas. In this study, the authors evaluated sustainability through the analysis of five case studies of practical use of nZVI in field-scale remediation in different locations around the world. In this study, the authors found that the case study in Brazil was the one with the lowest sustainability compared to the case studies of China, Spain, Hungary and the United States. Based on the results verified In Chapter IV it was verified the gap of a more detailed analysis on the feasibility of use in nZVI in the remediation of contaminated areas in Brazil.

Thus, this article has as main objective to verify the feasibility of the use of nZVI in the remediation of contaminated soils, from a perspective of Brazil. While the specific objectives are: (i) to analyze the environmental, economic and social viability of different remediation techniques through life cycle analysis tools; (ii) determine which remediation technique is more sustainable for use in Brazil in the scenarios considered (unsaturated soil and saturated soil); (iii) to evaluate the Brazilian perspective for the use of nanoremediation with nZVI in soil and groundwater remediation. It is noteworthy that this work does not aim to verify the efficiency of the selected remediation techniques, only their sustainability.

2. Methodology

2.1 Description of contaminated site

For this study, an area located in southern Brazil was selected. Soil characteristics information was taken from Reginatto et al. (2020b). This site presents contamination with hexavalent chromium, both in an unsaturated zone and in the saturated zone. The soil of the site is a claysoil composed of 72% clay, 15% silt and 13% sand. This is a tropical, structured residual soil, and kaolinite is the predominant clay mineral, which confers the characteristic of greater permeability in relation to unstructured clay soils. The hydraulic conductivity of the soil is 1.39×10^{-3}cm/s (Reginatto et al. 2020b).

Two contamination scenarios were defined for the analysis:

- • **Scenario I - Unsaturated soil:** For scenario I, only unsaturated soil remediation was considered. The concentration of chromium at the site is 100 mg/kg. The intervention value for this contaminant in Brazil for residential areas is 3.2 mg/kg, in the United States the intervention value for residential soils is 0.3 mg/kg, and in the Netherlands standard the value is 7.8 mg/kg. The size of the contaminated area is 2 m x 5 m, and the plume lies at a depth of 4 meters. The volume to be remedied was estimated at 10 m^3.

- • **Scenario II - Saturated soil:** For scenario II was considered only the remediation of saturated soil. The concentration of chromium at the site is 50 mg/L (Reginatto et al. (2020b). The intervention value of Brazil for the remediation of groundwater contaminated with this type of contaminant is 50 μg/L, in the United States it is 0.1 mg/L, and in the European Union 2 mg/L (Tumolo et al. 2020). The size of the contaminated area was estimated at 2m x 5m, and the plume is at a depth of 10 meters. The volume to be remedied was estimated at 10m^3.

2.1.1 Remediation Techniques

The remediation techniques were selected considering the type of contaminant and the characteristics of the soil to be remedied. In addition, we sought to select the most used techniques in the remediation of Brazil. Thus, Table V - 1 shows the selected techniques and a description of operation and remediation efficiency.

The efficiency of remediation was described according to the data reported in the literature in studies that used the techniques. In this work, a field pilot analysis was not performed to determine the efficiencies in the data of this case study. This study seeks to perform an initial theoretical analysis to verify the feasibility of the use of nZVI in remediation, and comparing the results obtained with techniques applied in chromium remediation in scenarios considering the situation of the remediation market in Brazil, such as the availability of the technique and also selecting the most used techniques in the country.

Table V - 1: Remediation techniques selected, description and efficiency.

Remediation technique	**Description**	**Efficiency reported in the literature for Cr (VI) remediation**
Chemical oxy-reduction	It considers the oxidation and reduction potential of certain chemical compounds to promote a chemical transformation of the contaminant through oxireduction reactions (Gao et al. 2022). The remediation process occurs through in situ injection of the reagent into the contaminated area. In the case of hexavalent chromium, reagents are used that perform the reduction to trivalent chromium, a less toxic compound (Franco et al. 2009). It can be used in the remediation of unsaturated soils and also saturated soils.	60 a 99% (U.S EPA, 2004; 2005a; 2018).
Soil washing	It is used in the remediation of saturated and unsaturated soils. It has two settings according to the form of use, whether in situ or ex situ. The washing of ex situ soils initially occurs the excavation of contaminated soil, after it is transferred to the remediation station, where it is initially sieved (Liu et al 2021). The finer particles in the soil are discarded in landfill. While the coarser particles are washed away. Clean soil can be re-destined to the area. In many cases there is a need to dig clean soil from other sites to target the remediated area. In situ soil washing is referred to as in situ flushing. In this technique is made the injection or spraying of water or an aqueous solution in the contaminated area, with this occurs the leaching of water and contaminant to the groundwater (Liu et al. 2021). With extraction well the groundwater is collected and destined for treatment.	60 a 90 % (U.S. EPA, 1990; Xuan et al. 2016).

Remediation technique	Description	Efficiency reported in the literature for Cr (VI) remediation
Stabilization and solidification	It consists of reducing the mobility of contaminants through the addition of agglomerates and physical processes (Wang et al. 2021). Remediation occurs by injecting or mixing the stabilizing agents into a subsurface to immobilize the contaminant and prevent its leaching into groundwater (Conner, Hoeffner, 1998). The main material used in this process is cement.	90 to 99% (Wang et al. 2021; Silva et al. 2021).
Nanoremediation	Nanoremediation is nothing more than a chemical reduction technique using nanomaterials (Thomé et al. 2015). The process usually occurs through in situ injection of the nanomaterial into the contaminated area (Thomé et al. 2015).	50 to 98 % (Cecchin et al. 2021; Reginatto et al. 2020).
Excavation and disposition	It is not considered as a remediation technique, but it is widely used. In this process occurs the excavation of contaminated soil and destination of this to an industrial landfill. There is also the excavation of clean soil for replacement of excavated soil (Amponsah et al. 2018).	It is not a remediation technique, so efficiency is not evaluated as in other techniques.
Pump and Treat	It is the most common technology used for groundwater remediation. The remediation system involves pumping groundwater to the surface, removing contaminants, and recharging treated water underground or discarding it (Bortone et al. 2020).	40 to 87 % (U.S.EPA, 2005b)

2.2 Viability analysis

The viability analysis was performed considering the methodology of life cycle analyses. Thus, four life cycle analyses were performed, according to the methodology of Visentin et al. (2021a): life cycle analysis (LCA), life cycle costs (LCC), Social life cycle analysis (S-LCA) and Life Cycle Sustainability Analysis (LCSA). Next, the methodological procedure for life cycle analyses is detailed. As all analyses follow ISO 14.040 (2006) the methodology will be presented together of all analyses, only in the stage of analysis of impacts will be made a separate description for each analysis of the life cycle, since not all analyses have the same degree of maturity in its use, because, while the LCA is the most known and used methodology, S-LCA and LCSA do not yet have a universal method (Visentin et al. 2020).

2.2.1 Goal and scope definition

The goal of life cycle analyses is to assess the environmental, economic, social and sustainability impacts of the different remediation techniques defined and described in Section 2.1.1. The intended application of the analyses is to verify whether, from the point of view of life cycle sustainability, the use of nZVI in the remediation of saturated and unsaturated soils is sustainable in Brazil. The target audience is researchers in the area of sustainable remediation and decision makers. The functional unit of the life cycle analyses was 10.00 m³ of soil and remediated groundwater. This functional unit was selected in order to allow comparison between the different remediation techniques.

2.2.2 Inventory analysis

The inventory of remediation techniques was made with secondary data obtained in publications that used the techniques considered in this study, and data from similar processes. Estimates were made in order to adjust the data for the functional unit of this study, and also considering the concentration of contamination.

Table V - 2 presents the inventory of remediation techniques in relation to environmental and economic aspects, and the references used for the inventory. Social inventory is based on country-level data, on global reports, and also on the operational characteristic of each technique. The social inventory is presented in the Supplemental Material.

Table V - 2: Environmental and economic inventory of remediation techniques.

Remediation techniques	Stages	Inputs and outputs	Amount	Costs
In situ chemical reduction/ oxidation (Scenario I)	Site preparation	PVC pipes	12 m	20.34 $/m
		Excavation	1 h	100 $/h
		Transport truck	60 km	13.10 $/km
		Solid waste	90 kg	380.00 $/ton
	Remediation	Heptahydrate iron sulfate	35.02 kg	166.00 $/kg

		Deionized water	166 m³	3.00 $/m³
		Energy	2.325 kWh	0.16 $/kWh
		Transport truck	1014 km	13.10 $/km

Remediation techniques	**Stages**	**Inputs and outputs**	**Amount**	**Costs**
In situ chemical reduction/ oxidation (Scenario I)	Monitoring	Energy	0.9 kWh	0.16 $/kWh
		Wastewater	8 $x10^{-3}$ m³	0.15 $/m³
		Solid waste	0.2 kg	380.00 $/ton
	Labor costs	Excavation	1 h	10.70 $/h
		Remediation	8.5 h	60.00 $/h
Soil washing (Scenario I)	Site preparation	Excavation	4 h	100 $/h
		Transport truck	5 km	13.10 $/km
	Remediation	Water	29.18 m³	3.00 $/m³
		Energy	428 kWh	0.16 $/kWh
		Activate carbon	100 kg	20.00 $/kg
		Solid waste	1148 kg	380.00 $/ton
		Transport truck	120 km	13.10 $/km
		Wastewater	8 $x10^{-3}$ m³	0.15 $/m³
		Excavation	2 h	100 $/h
	Monitoring	Energy	0.45 kWh	0.16 $/kWh
		Wastewater	8 $x10^{-3}$ m³	0.15 $/m³
		Solid waste	0.2 kg	380.00 $/ton
	Labor costs	Excavation	6 h	10.70 $/h
		Remediation	11 h	60.00 $/h
Nanoremediation with comercial nZVI (Scenario I)	Site preparation	PVC pipes	12 m	20.34 $/m
		Excavation	1 h	100 $/h
		Transport truck	60 km	13.10 $/km
		Solid waste	90 kg	380.00 $/ton
	Remediation	nZVI (NANOFER STAR ®)	219.5 kg	6.00 $/kg
		Deionized water	0.65 m³	3.00 $/m³
		Energy	2.325 kWh	0.16 $/kWh
		Transport airplane	11151 km	4.50 $/kg
		Transport truck	288.7 km	13.10 $/km
	Monitoring	Energy	0.9 kWh	0.16 $/kWh
		Wastewater	8 $x10^{-3}$ m³	0.15 $/m³
		Solid waste	0.2 kg	380.00 $/ton
	Labor costs	Excavation	0.5 h	10.70 $/h
		Remediation	10 h	60.00 $/h

Remediation techniques	Stages	Inputs and outputs	Amount	Costs
Stabilization and solidification (Scenario I)	Remediation	Cement	3.200 kg	2.79 $/kg
		Water	1.6 m³	3.00 $/m³
		Energy	460 kWh	0.16 $/kWh
		Transport truck	120 km	13.10 $/km
	Monitoring	Energy	0.9 kWh	0.16 $/kWh
		Wastewater	8 x10^{-3} m³	0.15 $/m³
		Solid waste	0.2 kg	380.00 $/ton
	Labor costs	Excavation	3 h	10.70 $/h
		Remediation	6 h	60.00 $/h
Excavation and landfill disposal (Scenario I)	Remediation	Excavation	8 h	100 $/h
		Transport truck	240 km	13.10 $/km
		Solid waste	16 ton	380.00 $/ton
	Monitoring	Energy	0.45 kWh	0.16 $/kWh
		Wastewater	8 x10^{-3} m³	0.15 $/m³
		Solid waste	0.2 kg	380.00 $/ton
	Labor costs	Excavation	8 h	10.70 $/h
		Remediation	10 h	60.00 $/h
Nanoremediation using nZVI produced on site by green synthesis (Scenario I)	Site preparation	PVC pipes	12 m	20.34 $/m
		Excavation	1 h	100 $/h
		Transport truck	60 km	13.10 $/km
		Solid waste	90 kg	380.00 $/ton
	Remediation	Leaves	38.86 kg	21.90 $/kg
		Iron chloride (III) - $FeCl_3$	636.55 kg	41.60 $/kg
		Deionized water	11 m³	3.00 $/m³
		Energy	3.01 kWh	0.16 $/kWh
		Transport truck	1014 km	13.10 $/km
	Monitoring	Energy	0.9 kWh	0.16 $/kWh
		Wastewater	8 x10^{-3} m³	0.15 $/m³
		Solid waste	0.2 kg	380.00 $/ton
	Labor costs	Excavation	0.5 h	10.70 $/h
		Remediation	10 h	60.00 $/h

Remediation techniques	Stages	Inputs and outputs	Amount	Costs
In situ chemical reduction/ oxidation (Scenario II)	Site preparation	PVC pipes	20 m	20.34 $/m
		Excavation	1 h	100 $/h
		Transport truck	60 km	13.10 $/km
		Solid waste	270 kg	380.00 $/ton
	Remediation	Heptahydrate iron sulfate	3.30 kg	166.00 $/kg
		Deionized water	5 m³	3.00 $/m³
		Energy	2.325 kWh	0.16 $/kWh
		Transport truck	1014 km	13.10 $/km
	Monitoring	Energy	0.9 kWh	0.16 $/kWh
		Wastewater	8×10^{-3} m³	0.15 $/m³
		Solid waste	0.2 kg	380.00 $/ton
	Labor costs	Excavation	0.5 h	10.70 $/h
		Remediation	18 h	60.00 $/h
In situ flushing (Scenario II)	Site preparation	PVC pipes	20 m	20.34 $/m
		Excavation	1 h	100 $/h
		Transport truck	60 km	13.10 $/km
		Solid waste	270 kg	380.00 $/ton
	Remediation	Heptahydrate iron sulfate	3.30 kg	166.00 $/kg
		Deionized water	5 m³	3.00 $/m³
		Activate carbon	200 kg	20.00 $/kg
		Energy	189 kWh	0.16 $/kWh
		Transport	1014 km	13.10 $/km
	Monitoring	Energy	0.9 kWh	0.16 $/kWh
		Wastewater	8×10^{-3} m³	0.15 $/m³
		Solid waste	0.2 kg	380.00 $/ton
	Labor costs	Excavation	0.5 h	10.70 $/h
		Remediation	70 h	60.00 $/h
Nanoremediation with comercial nZVI (Scenario II)	Site preparation	PVC pipes	20 m	20.34 $/m
		Excavation	1 h	100 $/h
		Transport truck	60 km	13.10 $/km
		Solid waste	270 kg	380.00 $/ton
	Remediation	nZVI (NANOFER STAR ®)	0.0010 kg	6.00 $/kg
		Deionized water	0.65 m³	3.00 $/m³
		Energy	2.325 kWh	0.16 $/kWh
		Transport airplane	11151 km	4.50 $/kg
		Transport truck	288.7 km	13.10 $/km

Remediation techniques	Stages	Inputs and outputs	Amount	Costs
Nanoremediation with comercial nZVI (Scenario II)	Monitoring	Energy	0.9 kWh	0.16 $/kWh
		Wastewater	8 x10^{-3} m³	0.15 $/m³
		Solid waste	0.2 kg	380.00 $/ton
	Labor costs	Excavation	0.5 h	10.70 $/h
		Remediation	8.5 h	60.00 $/h
Pump and treat (Scenario II)	Site preparation	PVC pipes	20 m	20.34 $/m
		Excavation	1 h	100 $/h
		Transport truck	60 km	13.10 $/km
		Solid waste	270 kg	380.00 $/ton
	Remediation	Energy	1.493.1 kWh	0.16 $/kWh
		Activate carbon	200 kg	20.00 $/kg
		Transport	1014 km	13.10 $/km
		Solid waste	500 kg	380.00 $/ton
	Monitoring	Energy	1.8 kWh	0.16 $/kWh
		Wastewater	8 x10^{-3} m³	0.15 $/m³
		Solid waste	0.2 kg	380.00 $/ton
	Labor costs	Excavation	0.5 h	10.70 $/h
		Remediation	490 h	60.00 $/h

2.2.3 Impact assessment

- Environmental - Life cycle assessment. LCA was conducted in the SimaPro program through a Faculty license. The impact analysis methodology selected was Impact 2002+. This is the most widely used methodology in publications on LCA and nanomaterials.
- Economic - Life cycle costs. The LCC was also performed in the SimaPro program through the elaboration of a method of cost analysis, as detailed in previous studies (Visentin et al. 2019). Internal costs related directly to the remediation process (energy, raw materials, fuel, transportation, etc.) were evaluated, as well as external costs corresponding to the environmental costs resulting from the environmental impacts of remediation techniques (according to LCA results).
- Social life cycle assessment. The S-LCA was performed according to the adaptation of the methodology of Hossain et al. (2018) and detailed in Visentin et

al (2021b). This methodology is based on calculations that relate social indicators with midpoint and endpoint impact categories, and with this a social index of the life cycle can be determined.

2.2.4 Sustainability analysis

- • Life cycle sustainability asssessment. LCSA was performed through a multicriteria analysis methodology, as presented in a previous study in Visentin et al. (2021a). The sustainability index of the life cycle is calculated by summing up the normalized scores of environmental, economic and social impacts, and also based on a weighting factor. In this study, the weighting factor was considered equal to 1.00 with equal importance the categories of impact and aspects of sustainability. Visentin et al. (2021a) found that the use of weighting factors compared to weighting equal to 1.00 does not result in significant differences in the sustainability index.

3. Results and Discussion

3.1 Environmental viability

The environmental viability of remediation techniques was evaluated in the LCA. Figure V - 1 shows the total impacts of remediation techniques, and also in each impact category, in the two scenarios considered, scenario I unsaturated soil, and unsaturated soil scenario II. In all scenarios, impacts were considered for the functional unit of 10 m³ of remediated soil. Environmental impacts are expressed in mPt. The magnitude of this numerical value expresses the size of the global environmental impact, that is, the higher the value, the greater the environmental impact (Visentin et al. 2019). While Table V - 3 presents the impacts of the remediation steps of each technique.

Figure V - 1:Total environmental impacts and impact categories in the two scenarios considered.

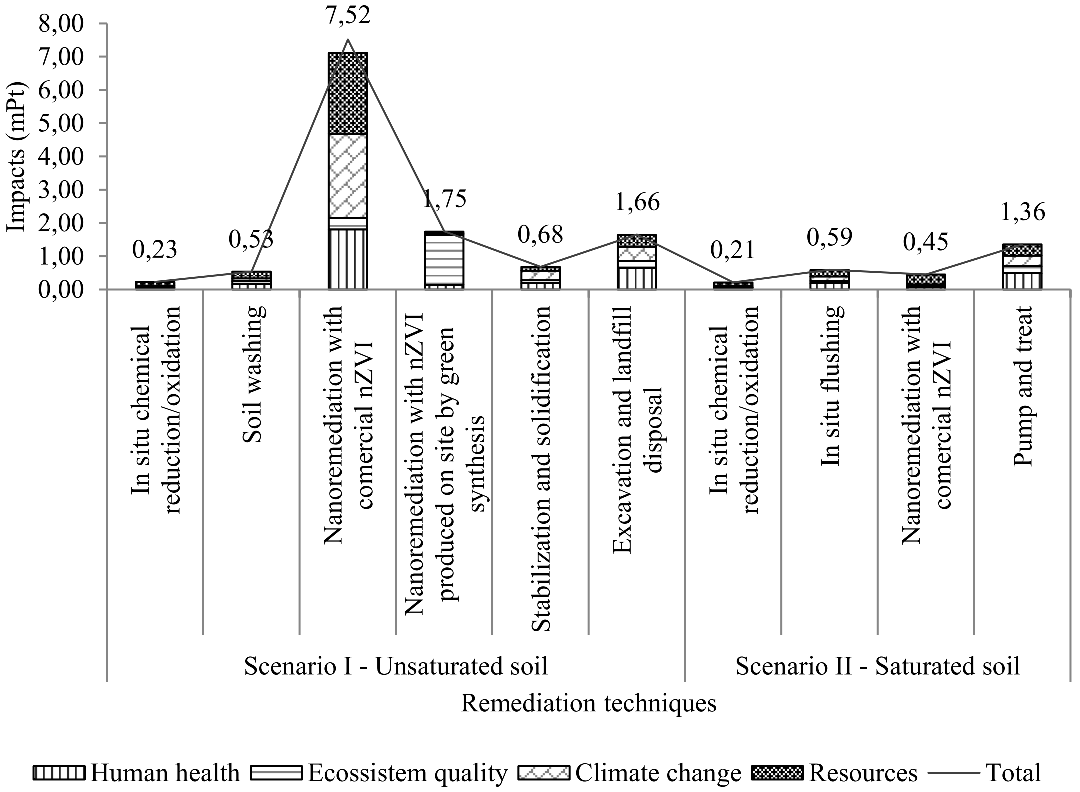


Table V - 3: Percentage contribution of each stage to the environmental impacts of remediation techniques in the two scenarios evaluated.

Scenario	Remediation techniques	Site preparation	Remediation	Monitoring	Disposal of landfill waste and/or wastewater treatment
Scenario I - Unsaturated soil	In situ chemical reduction/oxidation	10.1%	87.1%	0.1%	2.7%
	Soil washing	6.8%	70.4%	0.0%	22.8%
	Nanoremediation with comercial nZVI	0.1%	99.8%	0.0%	0.1%
	Stabilization and solidification	0.0%	98.9%	0.0%	1.1%
	Excavation and landfill disposal	0.0%	19.7%	0.0%	80.3%
	Nanoremediation using nZVI produced on site by green synthesis	0.9%	99.0%	0.5%	0.0%

Scenario	Remediation techniques	Site preparation	Remediation	Monitoring	Disposal of landfill waste and/or wastewater treatment
Scenario II - Saturated soil	In situ chemical reduction/oxidation	9.6%	82.7%	0.1%	7.7%
	In situ flushing	6.3%	61.0%	0.0%	32.7%
	Nanoremediation with comercial nZVI	0.1%	86.6%	8.2%	5.1%
	Pump and treat	0.0%	67.0%	0.0%	33.0%

In scenario I of unsaturated soil, the nanoremediation with commercial nZVI resulted in the greatest environmental impacts among the techniques considered, followed by excavation and landfilling. Soil washing and stabilization/solidification techniques resulted in similar impacts, while the chemical oxy-reduction technique resulted in the lowest environmental impacts.

For all techniques, the greatest impacts were verified in the remediation stage, which contains the materials used during the remediation process, such as nZVI, iron sulfate, activated carbon and also energy consumption. In the excavation and disposal, the greatest impacts were verified in the landfill stage of the contaminated soil. Highlighting the nanoremediation, the impacts are associated with the production of nZVI and the transport of this from the Czech Republic to Brazil. The impacts of nZVI production correspond to 88% of the total impacts of the technique, while transport at 11.6%.

In scenario II in saturated soil, the pump and treat technique resulted in the greatest environmental impacts, followed by the in situ flushing technique. In pump and treat the main factor contributing to the impacts is the remediation time, which is significantly higher compared to the other techniques. Oxyreduction and nanoremediation techniques resulted in the lowest environmental impacts. In the stages of application of the techniques, the impacts are mainly verified in the remediation stage. And in the techniques in situ flusing and pump and treat the stage of disposal of waste in landfill also contributes to the impacts.

Considering the technique of nanoremediation, in the evaluated scenarios of unsaturated and saturated soils, it is perceived that the technique is not environmentally feasible for use in unsaturated soil in terms of environmental impacts. This fact is due to the greater amount of nZVI used in unsaturated soils compared to saturated soils. The concentration of nZVI used in nanoremediation with commercial nZVI in scenario I was 12.5 mg/kg while the concentration of nZVI in scenario II was 10g/L (Zhang et al. 2019; Otaegi and Cagigal, 2017). The amount of nZVI used in remediation in scenario I was 219.5 kg, while in scenario II 10.9 g (Otaegi and Cagigal, 2017). According to Chapter IV, the amount of nZVI used in remediation is the main factor that influences the environmental impacts of the technique.

The nZVI considered in the nanoremediation technique consists of the commercial nZVI distributed by the company NanoIron ® located in the Czech Republic. In this context, there are the production impacts of the nZVI, as well as transport. Thus, in Scenario I, a change in the configuration of the technique, considering the on-site production of the nZVI by the green synthesis method significantly reduces the impacts of nanoremediation.

3.2 Economic viability

The economic viability of remediation techniques was evaluated through the LCC. Figure V - 2 shows the total life cycle costs for the two scenarios considered and also in the evaluated cost categories. The costs are expressed in U$/m³ of remediated soil. While Table V - 4 presents in detail the costs of each technique in the steps of remediation in terms of percentage.

Figure V - 2: Life cycle costs of remediation techniques in the evaluated scenarios.

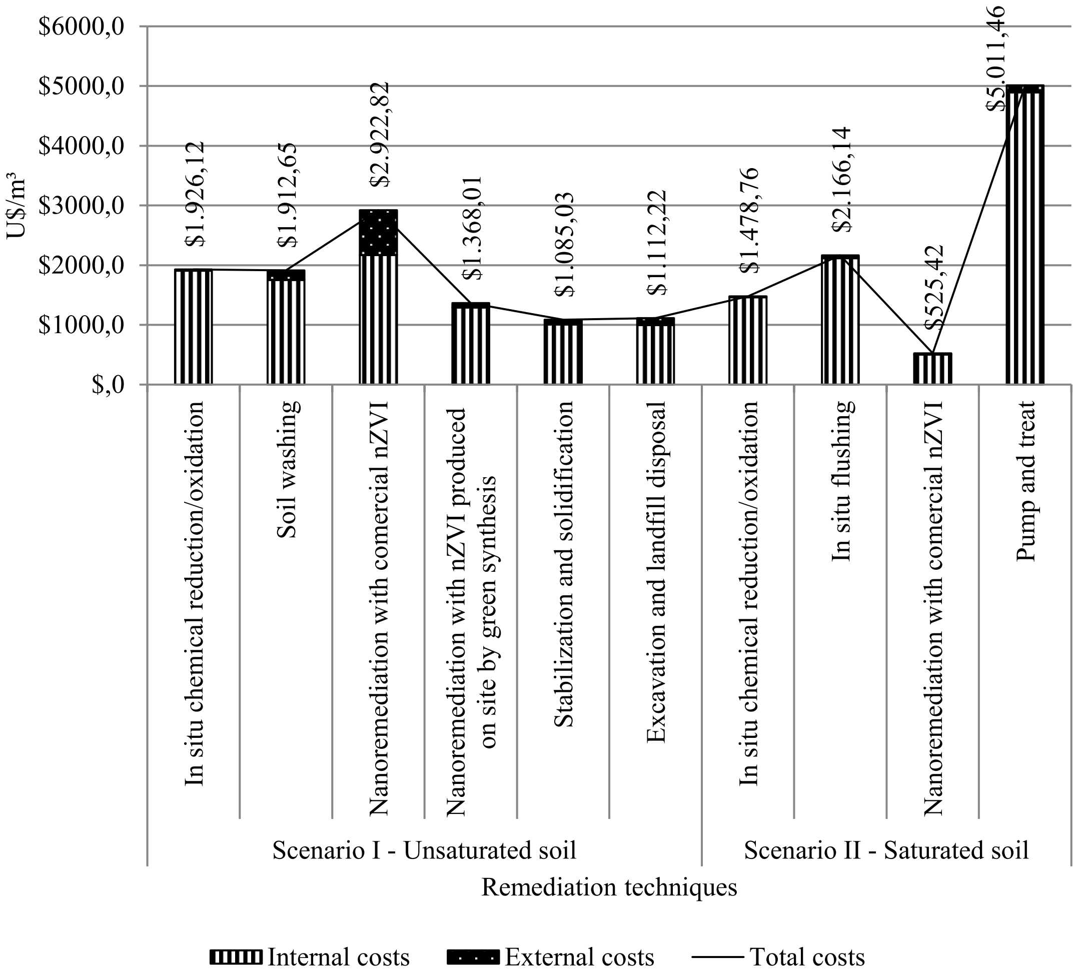


Table V - 4: Percentage contribution of each stage to the environmental impacts of remediation techniques in the two scenarios evaluated.

Scenario	**Remediation techniques**	**Site preparation**	**Remediation**	**Monitoring**	**Disposal of landfill waste and/or wastewater treatment**	**External costs**
Scenario I - Unsaturated soil	In situ chemical reduction/oxidation	5.1%	92.2%	1.7%	0.2%	0.8%
	Soil washing	2.2%	86.5%	0.8%	2.1%	8.3%
	Nanoremediation with comercial nZVI	3.3%	69.3%	1.1%	0.1%	26.2%

Scenario	Remediation techniques	Site preparation	Remediation	Monitoring	Disposal of landfill waste and/or wastewater treatment	External costs
Scenario I - Unsaturated soil	Stabilization and solidification	0.0%	89.5%	3.0%	0.0%	7.5%
	Excavation and landfill disposal	3.9%	20.7%	2.9%	61.9%	10.5%
	Nanoremediation using nZVI produced on site by green synthesis	7.1%	85.09%	2.3%	0.2%	5.0%
Scenario II - Saturated soil	In situ chemical reduction/oxidation	2.8%	88.6%	2.2%	5.4%	1.0%
	In situ flushing	1.9%	90.6%	1.5%	3.7%	2.3%
	Nanoremediation with comercial nZVI	7.9%	67.5%	6.2%	14.0%	4.4%
	Pump and treat	0.8%	93.9%	1.3%	1.6%	2.4%

In scenario I – unsaturated soil, the highest life cycle costs were verified in nanoremediation considering the commercial nZVI acquired in Nanoiron ®. In situ chemical oxidation/reduction and soil washing techniques have similar costs for remediation. The technique of nanoremediation considering the production at the nZVI site by the green synthesis method resulted in lower costs than the techniques already mentioned, having a cost similar to excavation and disposal. While the stabilization and solidification technique resulted in lower life cycle costs.

The costs of scenario I techniques mainly involve the internal costs of remediation, which are the costs of materials, transportation and energy. Labor costs also make a significant contribution to the costs of the techniques. The external costs corresponding to environmental costs are higher in the technique of nanoremediation with commercial nZVI, because this technique also resulted in the greatest environmental impacts of scenario I.

In scenario II – saturated soil, the highest costs are verified in the pump and treat technique, due to the longer remediation time, which results in operating costs such as energy and also labor costs. The in situ flushing technique resulted in the second highest cost of the life cycle of scenario II, followed by the in situ chemical oxidation/reduction technique. While the nanoremediation technique resulted in the lower lifecycle costs of scenario II.

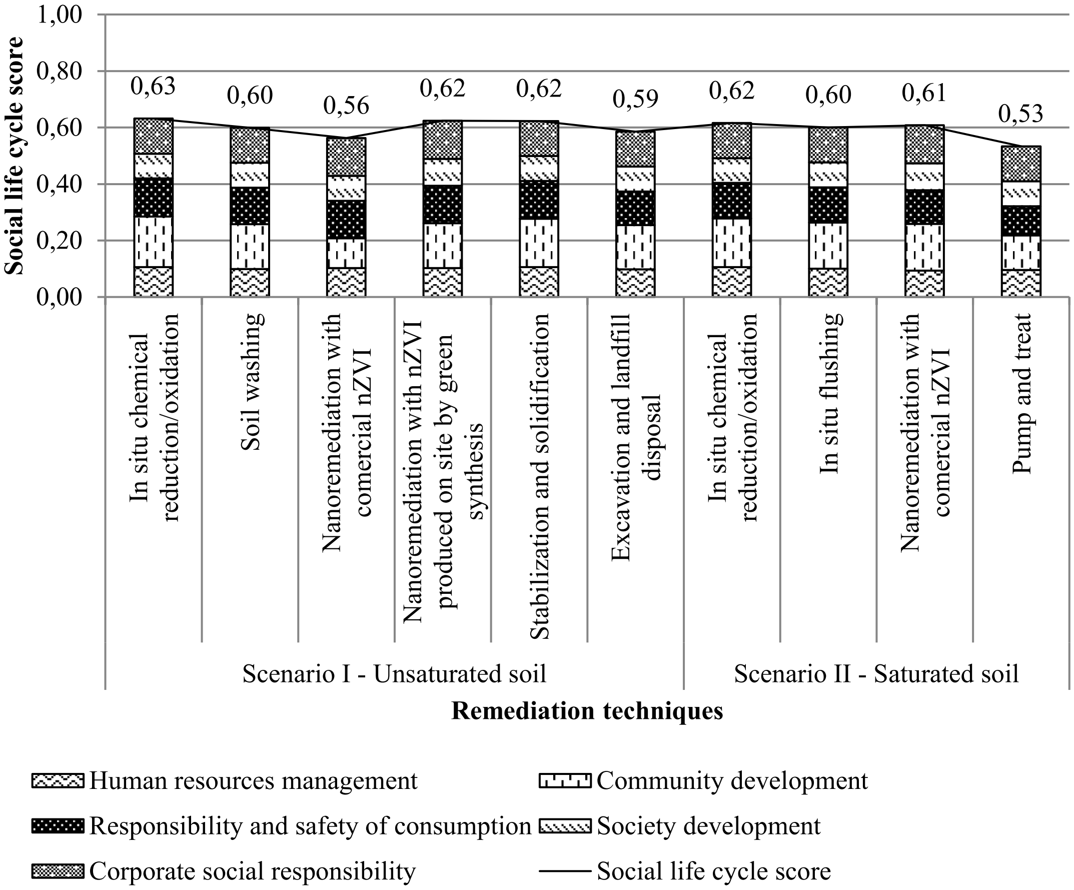
The costs of scenario II techniques also have a greater contribution to internal costs. For example, in pump and treat, labor costs account for 64.4% of the total costs of the technique. In situ flushing the greatest impact contributions are verified in the remediation stage, with costs of activated carbon, transportation and labor. In the technique of oxidation/chemical reduction in situ, transport costs have a higher contribution corresponding to 52.4% of the total costs. In nanoremediation, transport and labor costs correspond to 35.2% and 22.1%, respectively.

The difference in costs is perceived in comparison of nanoremediation techniques for unsaturated soils (scenario I) and saturated soils (scenario II). This fact occurs due to the lower amount of nZVI used in saturated soils. With this, it is verified that for unsaturated soils the use in nanoremediation may not be viable in economic terms. The production at the nZVI site by the green synthesis method improves the viability of the technique, resulting in costs similar to the other techniques evaluated for unsaturated soils.

3.3 Social viability

The social viability of remediation techniques was evaluated through S-LCA. Figure V - 3 presents the social life cycle score of each remediation technique in the two scenarios evaluated, also demonstrating the value in the impact categories. The value of the social life cycle score is dimensional, and its value ranges from 0.00 to 1.00, and the closer to 1.00 the more socially positive the technique.

Figure V - 3: Social life cycle score of remediation techniques in the evaluated scenarios.



In scenario I the highest value of the social life cycle score is the in situ chemical oxidation/reduction technique. The techniques of nanoremediation with nZVI produced on site by the method of green synthesis and stabilization and solidification resulted in social life cycle score of the same value (0.62). The soil washing technique and excavation and disposition resulted in a social life cycle score of 0.59. Finally, the lowest social life cycle score was in the nanoremediation technique with commercial nZVI.

In the categories of social impact, the lowest scores were verified in all techniques in the society development category. In this category, indicators involving the characteristics of the country of remediation are involved, in the case of Brazil. The values of the country's indicators in government reports are lower than in comparison with developing countries such as the United States, the United Kingdom, etc. (Visentin et al. 2021b). The greatest variability in the social score is verified in the local community category, in this category there are indicators that involve the operational characteristics of remediation techniques, such as exposure to chemicals and contaminants; health risks during the remediation process; health and safety measures.

In scenario II, the highest value of the social life cycle score was verified in the in situ chemical oxidation/reduction technique. Next is the nanoremediation technique and the flushing in situ technique. The lowest social life cycle score was verified in the pump and treat technique.

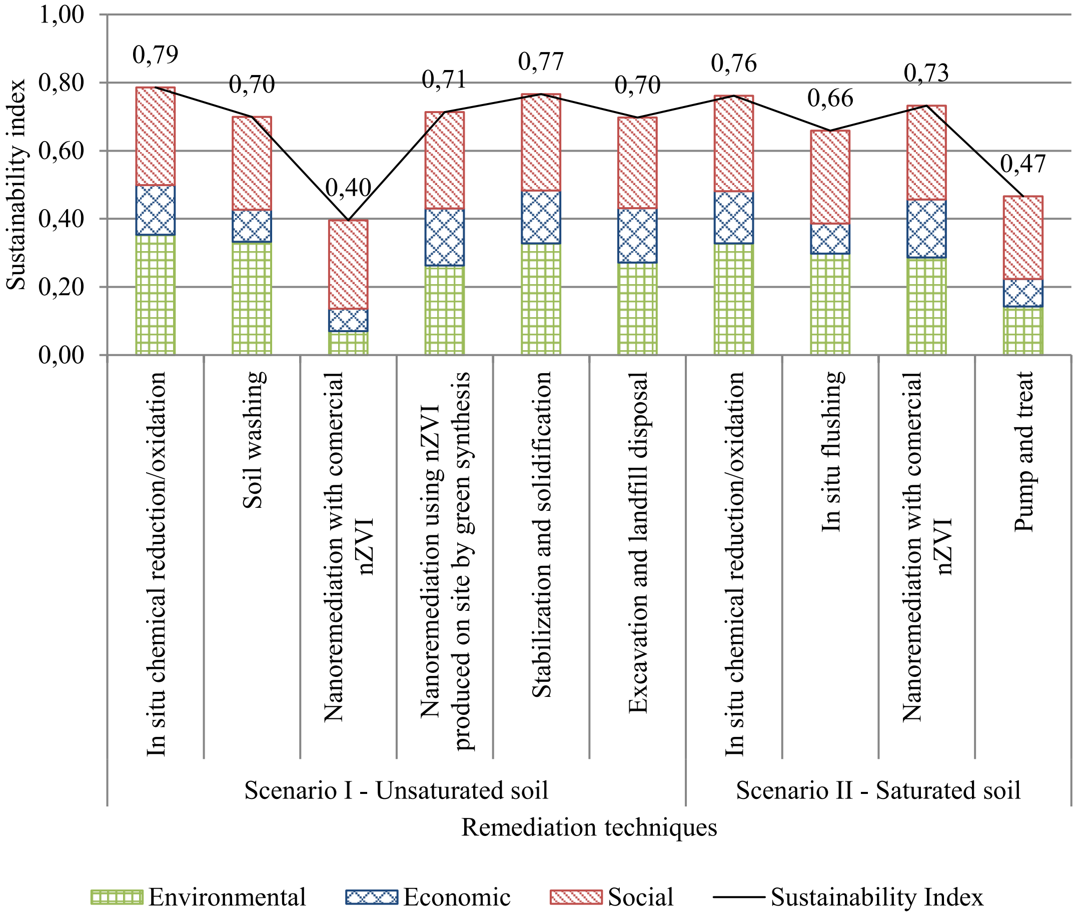
In the impact categories, the lowest scores were verified in the categories human resource manegement and society development. As in scenario I, the greatest variability of social scores in the impact categories was verified in the local community category.

In social terms, the difference between the social life cycle score is perceived in the nanoremediation technique for saturated and unsaturated soils. In scenario I of unsaturated soil, the social life cycle score was lower than compared to the technique in scenario II of saturated soil. And so it is perceived that nanoremediation is not socially viable. This fact is due to the operational characteristics of the techniques that have a difference in the amount of nZVI used that results in different impact scores on social indicators: exposure to contaminants (emission of gases that affect human health); quality of ecosystems; contribution to global warming; use of resources. The use of nZVI produced on site by the green synthesis method improves the social life cycle score of nanoremediation, making it more socially viable.

3.4 Sustainability

The sustainability of remediation techniques was evaluated through LCSA. Figure V - 4 presents the sustainability score of all techniques, highlighting the environmental, economic and social scores. The sustainability index is a dimensional index, and its value ranges from 0.00 to 1.00, and the closer to 1.00 the more sustainable the method. The sustainability classification was based on Visentin et al. (2021a).

Figure V - 4: Sustainability Index of remediation techniques in the evaluated scenarios.



For scenario I, the techniques of oxidation/chemical reduction in situ and stabilization / solidification resulted in the highest sustainability index, being classified as sustainable according to the classification presented in Visentin et al. (2021a). The techniques of nanoremediation with nZVI produced on site by the method of green synthesis, soil washing and excavation and disposal resulted in sustainability index of 0.71, 0.70 and 0.70, respectively, being also classified as sustainable. The technique of nanoremediation with commercial nZVI resulted in the lowest sustainability index of scenario I, being classified as unsustainable.

In the scenario II of saturated soils, the most sustainable technique was the in situ chemical oxidation/oxidation, followed by the technique of nanoremediation with nZVI, both classified as sustainable. The in situ flushing technique resulted in a sustainability index of 0.68, and was also classified as sustainable. The pump and treat technique resulted in the lowest sustainability index of all evaluated techniques, being classified as unsustainable.

The sustainability index is dependent on the environmental, economic and social performance of remediation techniques, according to results presented above. Thus, it is perceived that the techniques that resulted in greater environmental impacts and life cycle costs resulted in scores of these smaller categories compared to techniques with lower environmental impacts and costs. This case is perceived in the nanoremediation technique in scenario I, and in the pump and treat in scenario II. The social score was generally similar for all remediation techniques, with standard deviation of 0.03, and thus, few differences in the social score were verified in the sustainability index.

In general, nanoremediation with commercial nZVI is an unsustainable technique in scenario I for unsaturated soils. The modification of the nanoremediation configuration in scenario I considering the on-site production of the nZVI through the green synthesis method improves the sustainability of nanoremediation, with the sustainability index being 2x lower than in nanoremediation considering the commercial nZVI. On the other hand, the sustainability index of nanoremediation in scenario II was the largest verified in nanoremediation techniques. Thus, confirming all the viability results presented throughout the article, it is verified that the use of nZVI in the remediation of unsaturated soils is more sustainable than the use in unsaturated soils.

The sustainability of nanoremediation with nZVI is directly related to the amount of nZVI used in the remediation process. In scenario I of unsaturated soil, higher amounts of nZVI are required than in saturated soils (scenario II).

3.4.1 Efficiency vs. sustainability

An interesting analysis to be made is the comparison between the sustainability of remediation techniques with the efficiency in remediation. In this study, a pilot analysis was not made in order to determine the actual efficiency of each remediation technique in the area to be remedied and in the scenarios considered. Thus, considering the theoretical efficiency presented in the previously detailed literature, this comparative analysis can be performed, according to Table V - 5.

Table V - 5: Relationship between sustainability index and remediation efficiency.

Scenario	Remediation techniques	Sustainability Index	Sustainability Classification	Efficiency reported in the literature for Cr (VI) remediation
Scenario I - Unsaturated soil	In situ chemical reduction/oxidation	0.79	Sustainable	60 a 99% (U.S EPA, 2004; 2005a; 2018).
	Soil washing	0.70	Sustainable	60 a 90 % (U.S. EPA, 1990; Xuan et al. 2016).
	Nanoremediation with comercial nZVI	0.40	Unsustainable	50 a 98 % (Cecchin et al. 2021; Reginatto et al. 2020).
	Stabilization and solidification	0.77	Sustainable	90 a 99% (Wang et al. 2021; Silva et al. 2021).
	Excavation and landfill disposal	0.70	Sustainable	It is not a remediation technique, so efficiency is not evaluated as in other techniques.
	Nanoremediation using nZVI produced on site by green synthesis	0.71	Sustainable	60 a 95% (Afroosheh et al. 2021).
Scenario II - Saturated soil	In situ chemical reduction/oxidation	0.76	Sustainable	60 a 99% (U.S EPA, 2004; 2005a; 2018).
	In situ flushing	0.66	Sustainable	60 a 90 % (U.S. EPA, 1990; Xuan et al. 2016).
	Nanoremediation with comercial nZVI	0.73	Sustainable	50 a 98 % (Cecchin et al. 2021; Reginatto et al. 2020).
	Pump and treat	0.47	Unsustainable	40 a 87 % (U.S.EPA, 2005b)

In general, remediation techniques have high efficiencies (above 60%), which in many studies is already enough to achieve remediation goals. A fact that deserves to be highlighted is that nanoremediation with commercial nZVI in unsaturated soils (scenario I) presents a high efficiency, in many studies this efficiency is achieved in the first days of remediation. In this way, studies in this configuration are perceived in order to encourage the practical use of the technique. However, as verified throughout this article this is not a viable and sustainable technique in the remediation of unsaturated soils with commercial nZVI. While the use of nZVI produced on site by the green synthesis method results in a higher sustainability index and has efficiency above 60% in the reported studies.

On the other hand, the pump and treat technique that was widely used in remediation in the United States and is still widely used in Brazil resulted in the lower sustainability index of the techniques in scenario II of saturated soil. Allied to this, it has been that in clay soils the technique does not have an adequate efficiency, and in many cases does not achieve the remediation objectives.

Thus, it is perceived that there is an important scientific gap to be filled with future studies, which should seek to evaluate the relationship between the sustainability of remediation techniques with efficiency. In this process can be evaluated the best way to include efficiency in the calculation of sustainability, or also verify in pilot studies the practical efficiencies of techniques and thus evaluate sustainability in a more comprehensive way with the reality of the site.

3.5 Brazilian Perspective

As verified throughout the article, the use of nZVI in unsaturated soils is not feasible in environmental, economic and social terms, besides not being a sustainable method. On the other hand, its use for groundwater remediation is feasible and sustainable.

In Brazil, the use of nanoremediation occurs basically at the laboratory level or on a pilot scale for research. There are no government data reporting the use of nanoremediation in the remeasurement of contaminated areas in the country. While in several countries in the world there have been initiatives in the use of nanoremediation, in Brazil this does not occur. In addition, remediation in Brazil is based exclusively on the costs and availability of technology for remediation. This fact is verified by the main remediation techniques used in the country, such as multiphase extraction, pump and treat, free phase recovery, excavation and disposal, chemical oxidation, vapor extraction, etc. (CETESB, 2020).

Considering the costs of the life cycle, nanoremediation with nZVI would be feasible only for use in groundwater remediation in Brazil, since this is a decisive factor in the choice of remediation technique. Allied to this, it is also found that nanoremediation results in shorter remediation times, which could make the technique feasible to be used in the country. Compared to the pump and treat technique, most used in Brazil, nanoremediation with nZVI in saturated soils results in lower environmental impacts and costs, and higher social index, besides being more sustainable.

The concern with environmental, social impacts and sustainability in the choice of remediation techniques is not yet a determining factor in many developed countries. In Brazil, there is no prospect of considering the aspects of sustainability as a decision-making factor in the choice of the remediation technique to be used (Braun et al. 2020b). Thus, the perspective for the use of nanoremediation in Brazil is not very encouraging, walking slowly, with a perspective still focused on research. However, this study found that the use of nanoremediation with nZVI is feasible to be used in Brazil in groundwater remediation, resulting in lower costs when compared to the pump and treat technique traditionally used.

4. Conclusion

In this article, an analysis of the feasibility of the use of nZVI in the remediation of contaminated areas was performed, and for this, two remediation scenarios were defined in an area located in the southern region of Brazil (scenario I - unsaturated soil and scenario II - saturated soil). Remediation techniques were defined for each scenario in order to compare viability through the analysis of environmental, economic, social and sustainability impacts with the nanoremediation technique.

Nanoremediation with commercial nZVI is not feasible for use in the remediation of unsaturated soils in Brazil (scenario I). The environmental impacts and costs were significantly higher in the technique of nanoremediation with commercial ZVI compared to other techniques for unsaturated soils and also compared with the technique in saturated soils (scenario II). In addition, the social index was lower in nanoremediation with commercial nZVI in scenario I. The sustainability of nanoremediation with commercial nZVI in scenario I of unsaturated soil was significantly lower than all other techniques, being classified as unsustainable. The alternative of using the nZVI produced on site by the green synthesis method improves in all aspects the viability of nZVI, making this technique sustainable for use in unsaturated soils.

From the perspective of Brazil, nanoremediation is feasible for use only in the remediation of saturated soils, due to lower costs compared to the pump and treat technique traditionally used.

The amount of nZVI used in remediation is the main factor that affects the viability and sustainability of its use in remediation. In saturated soils, according to the analysis of previous studies, the amount of nZVI required for remediation considering the same functional unit is significantly higher than that used in saturated soils. In this sense, there is also a scientific gap that can evaluate this need for a greater amount of nZVI in the remediation of unsaturated soils than in saturated soils.

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5. CAPÍTULO VI (artigo de resultados – não submetido): Life cycle sustainability assessment aggregating methods: a literature review, applications and a proposal for a composite sustainability index

Abstract: Life cycle sustainability analysis (LCSA) is a way to assess the sustainability of products, services and organizations in a lifecycle context. In this sense, the aim of this article is to propose a optimized LCSA aggregation method called composite sustainbility index. Thus, this study was initially carried out through a bibliometric research of LCSA publications, focusing on studies that applied aggregation methods. The methods of aggregation of the studies were identified, quantified and applied in data from a case study. In addition, the normalization and weighting methods were also evaluated. To determine the most complete method of aggregation of LCSA, a criterion analysis was performed through the participation of LCSA researchers, these criteria were validated and based on the preference score was made the ranking of the aggregation methods. The proposal of an LCSA aggregation method was carried out considering the most complete methods evaluated using the criteria. A total of 17 different methodologies were identified to aggregate the results of life cycle analyses, with different advantages and disadvantages. In the application of aggregation methods in a case study it was found that the results are varied, with a predominant sustainability classification. Among the criteria for selecting aggregation methods, LCSA researchers' preference is for methods that consider uncertainties and allow the participation of stakeholders. Finally, the proposed method is a composite sustainbility index that results in the optimization of the most complete methods. Thus, this study fills an important scientific gap, through the proposal of an optimized LCSA method. In addition, this study presents never-before-published approaches: analysis of all LCSA aggregation methods and application, analysis of selection criteria of LCSA aggregation methods with the participation of the main researchers in the area.

Key-words: Sustainability evaluation; Sustainability assessment; Multicriteria decision methos; Uncertainties; stakeholders participation.

1. Introduction

Sustainable development is becoming increasingly important to support the decision-making of business and government policies (Rodrigues et al. 2020). One example is the Sustainable Development Goals (SDG) of the 2030 Agenda for Sustainable Development. 17 DGSs have been defined which are global targets with priorities and aspirations to achieve sustainable development by 2030. The SDGs cover several areas, to integrate issues related to sustainable development into the general economic, environmental and social structures of its signatories (Caiado et al. 2018; Salvia et al. 2019).

For sustainable development to be implemented effectively, sustainability assessment measures are needed. And in this context there is the Life Cycle Sustainability Assessment (LCSA) as a way of assessing the sustainability of products, services and organizations in a life cycle context (Wafa et al. 2022). LCSA was originally structured according to the three pillars of sustainability and respective life cycle analyses, i.e., Life Cycle Assessment (LCA) (LCA) (ISO 14040: 2006; ISO 14044: 2006), Life Cycle Cost (LCC) (SETAC 2011) and Life Cycle Social Assessment (S-LCA) (UNEP 2009, 2020) (Kloepffer 2008).

LCSA is defined based on an operational sum relationship approach between LCA, LCC and S-LCA (Kloepffer 2008). In this approach, the three methods of life cycle analysis are performed separately for the same object of study and then their results can be compared individually or even, they can be aggregated with or without weighting in a life cycle sustainability score (Valdívia et al.2021). LCSA's innovative and holistic approach through the Triple Bottom Line (TBL) allows a systematic analysis of the environmental, social and economic dimensions of sustainability (Lassio et al. 2021). In 2011 the Life Cycle Initiative promoted a pragmatic LCSA structure that was adopted by the community in the form of numerous studies and articles of diversified geographical and sectoral origin (UNEP, 2011; Visentin et al. 2020).

The sustainability assessment requires not only an adequate assessment of each individual dimension of sustainability, but also the simultaneous consideration of each of them (Navaro et al. 2020). Thus, over the years LCSA research has focused on the application of life cycle analyses in different products and services, comparing the individual results of the analyses and also the development of aggregation methods. The assessment of LCSA sustainability is based on diverse and often conflicting criteria, for this fact, the main methods used in the aggregation of LCSA results are the Multicriteria Decision-Making Methods (MCDM) (Navaro et al. 2020, Visentin et al. 2020, Fetanat et al. 2022).

Multicriteria analysis is a decision-making process that uses the application of criteria in choosing the alternative closer to the ideal (Ren et al. 2017). These methods are mathematical tools used in solving decision-making problems in which they cover conflicting criteria (Yalcin et al. 2022). Multicriteria analysis can be divided into two types: (1) multi-objective decision-making (or multi-objective optimization), which works with an indefinite set of possible scenarios. It usually aims to optimize multiple objective functions with several particular constraints or without restrictions; and (2) MCDM (or multi-attribute decision analysis) suggests a finite set of scenarios. It usually aims to prioritize a finite set of alternatives with the consideration of multiple criteria (Ren et al. 2015).

LCSA advantage is transparency and identification of potential trade-offs between the three pillars of sustainability, such as lower emissions, but high production costs and fair wage (Backers and Traverso, 2021). However, some difficulties are observed in the use of LCSA, such as that the methods of life cycle analysis have different levels of data availability and maturity. This fact is related to the ease of use of the tools, methodological questions about the phase of impact assessment, interpretation of results (Valdivia et al. 2021). While LCA is the most well-known and standardized method, LCC and S-LCA are not yet standardized, which results in greater methodological variations in the applications of the studies (Visentin et al. 2020).

In addition, to date there is no universal LCSA method accepted by the scientific community. This gap has been highlighted in numerous studies. Valdívia et al. (2020) highlight that the LCSA structure is globally accepted and the need for an applicable approach is constantly increasing. Gubbert (2017) argues that LCSA needs an explicit and standardized way to integrate preferences into environmental, social and economic impact categories. Alejandrino et al. (2021) highlight the need to strengthen methodological trade-offs and obtain a consistent basis for future LCSA case studies. Therefore, methodologies are needed to promote the aggregation of life cycle analysis results in LCSA in a simple and guiding way, in order to improve decision-making in the sustainability of products, services and processes (Visentin et al. 2020).

Thus, the aim of this study is to propose a optimized LCSA aggregation method called composite sustainbility index. To this end, some specific objectives were outlined: (i) to analyze LCSA aggregation methods; (ii) application of aggregation methods in a case study and; (iii) analysis of criteria, validation and ranking of LCSA aggregation methods.

2. Methodology

2.1 Selection of LCSA methodologies

The selection of methodologies for analysis was based on detailed studies in Visentin et al. (2020) with methodologies that generate a unique sustainability score, aggregating the results of environmental, economic and social life cycle analyses.

Thus, in Visentin et al. (2020) 24 articles were detailed that used different methodologies to aggregate the results. Detailed articles in Visentin et al. (2020) comprise the time period from 2008 until the end of 2019.

A new analysis of publications was carried out in order to verify the studies published in the years 2020 to 2022 that used methodologies to aggregate results and define a single sustainability score. Thus, a new research was carried out in different databases (Scopus, Web of Science, Google Scholar, etc.) using the keywords: "Life cycle sustainability assessment" and "LCSA" according to the methodology of Visentin et al. (2020).

This research resulted in a total of 71 articles published in peer-reviewed journals from 2020 to 2022 to August 8, 2022. In these articles, a content analysis was performed in order to verify the type of article (review articles were not considered) and the methodologies used by the studies to evaluate the LCSA. The selected articles were those that performed an aggregation of environmental, economic and social results in a single sustainability score. After this analysis, 25 articles were considered in the analysis of methodologies.

With this, in the end, 49 articles were considered for the analysis of methodologies for aggregating the results of life cycle analyses into a sustainability score. In the Supplementary Material is presented the list of all articles considered in this study.

2.2 Analysis of aggregation methods

Initially, a quantitative analysis of the articles was made in order to catalog the articles regarding the aggregation method used, and when the weighting and normalization methods were applied. In addition, a critical analysis of the methods was made, according to the methodology of Rampanelli et al. (2021), highlighting the main points of its practical use to aggregate the results of life cycle analyses into a sustainability score. This analysis will be based on the facilities and difficulties that were observed during the use of the method in the case study. For each step of the method, the facilities and difficulties encountered were listed. This step aims to assist in the better understanding of the method, in order to verify the main difficulties and improvements to improve the practical use of the method.

2.3 Application of aggregation methods - case study

The methods of aggregation of the results of the selected life cycle analyses were applied in a case study by Chapter IV. In this study, the authors performed the analysis of the sustainability of the life cycle of the use of nano scale zero valente iron (nZVI) in the remediation of contaminated soils, through five case studies, which for this article were called Alternatives 1 to 5. LCA, LCC and S-LCA were performed to evaluate the impacts. And the sustainability score was obtained using the Multi-Attribute Value Theory (MAVT) method.

Briefly, the evaluated alternatives correspond to different practical uses in nZVI in remediation. Alternatives 1 and 2 correspond to the use in the remediation of soils not saturated with nZVI, being respectively in areas in Brazil and China. While alternatives 3, 4 and 5 correspond to remediation with nZVI in saturated soils, being respectively in areas in Spain, Hungary and the United States. More information about the data of each alternative can be verified in Visentin et al. (2023).

The results of the life cycle analyses of Chapter IV are presented in Table VI - 1.

Table VI - 1: Results of LCA, LCC and S-LCA by Visentin et al. (2022).

Life cycle analysis results	**Alternatives**				
Environmental impacts (mPt)	**A1**	**A2**	**A3**	**A4**	**A5**
Human Health	181.38	95.57	1.66	1.15	1.93
Quality of Ecosystems	33.86	76.60	0.52	0.34	0.53
Climate Change	254.71	17.52	1.36	1.04	1.30
Resources	242.70	20.04	1.66	1.12	1.42
Costs (U$/m³)					
Internal costs	761.01	2726.95	562.23	350.58	481.90
External environmental costs	416.28	43.27	2.55	2.88	2.40

Life cycle analysis results	Alternatives				
	A1	**A2**	**A3**	**A4**	**A5**
Social impacts (adimensional)					
Human Resources Management	0.1343	0.1352	0.1386	0.1338	0.1638
Community Development	0.0959	0.1280	0.1122	0.1326	0.1570
Responsibility and safety of consumption	0.1233	0.1258	0.1308	0.1308	0.1508
Development of society	0.1130	0.1426	0.1933	0.1859	0.1955
Corporate Social Responsibility	0.1011	0.1076	0.1149	0.1034	0.1588

The selected aggregation methods were applied with the data detailed above. All the steps of the aggregation method were followed, including the normalization method used. In the methods in which weighting weights were used, equal weighting weights were used to avoid deviations in the results due to differences in weighting weight values. Thus, it was possible to compare the sustainability results resulting from each method by varying only the aggregation method and the normalization method when applied. This analysis aims to verify the sustainability ranking of the alternatives resulting from each methodology, in order to analyze the differences between the results of each methodology.

The weighting weights used were 0.3333 for each aspect of sustainability (environmental, economic and social). Considering that in the case study data, each aspect of sustainability has different amounts of impact categories, a relationship was made. For example, for environmental aspects that have 4 categories of impact, the weighting value of each category was 0.3333/4 = 0.083325, for the economic categories the weighting value was 0.3333/2 = 0.16665, and for the social categories it was 0.33333/5 = 0.06666.

2.3.1 Analysis of criteria, validation and ranking of aggregation methods

The proposal of a LCSA method is based on the analysis of selection criteria of the aggregation methods used by decision makers. This step seeks to define which criteria are considered by decision makers in choosing the LCSA method to be used. In addition to the definition of criteria, the importance of these criteria was also quantified.

2.3.1.1 Definition of criteria

The selection criteria for the LCSA aggregation methods were initially made through the analysis of the LCSA methodologies defined in this study. Based on this analysis it was possible to determine an initial set of criteria that were considered by the studies. This initial analysis was performed through the knowledge and decision of the authors of this article. However, in the validation step of the criteria it was possible to add or modify the criteria initially defined.

2.3.1.2 Validation of criteria

The validation of criteria was performed through an online search through a questionnaire built on the Google Forms platform. The questionnaire consisted of three sections. The first section corresponded to the presentation of the questionnaire and the objectives. In the second section, the selection criteria for LCSA methods were considered. Six initial criteria were defined and the weighting of these was performed using the evaluation scale model (Likert). The third section requested some general information from the interviewees, such as country of origin; training and area of expertise; function, as well as data regarding LCSA methods already used by the interviewees, such as the number of methods used, proposed methods, importance of a LCSA method.

A 5-point Likert scale was used to assess the importance of the criteria. Scores range from 1 (irrelevant), 2 (not important), 3 (neutral), 4 (important) and 5 (very important), with 3 being the average value for acceptance of an indicator. Scale questionnaires are easier to understand and answer, and respondents more specifically indicate the degree of importance of each factor. A pilot questionnaire test was performed with approximately 10 researchers in the area of LCSA. Based on their comments, the questionnaire was reviewed and modified before being sent to the other participants.

The target population included specialists - researchers and professionals - in the area of LCSA. The size of the sample selected was due to the availability of members belonging to this target population to voluntarily respond to the available research. The survey was sent directly to 214 potential participants by email, with addresses collected in LCSA online publications. Repeated reminder emails were sent to encourage participation. We received 44 responses, resulting in a response rate of 21%, which can be considered satisfactory based on the specificity of the theme and is within the range normally obtained for this type of research, as observed in Braun et al. (2021), for example.

The results of the questionnaire were evaluated in spreadsheets. The analysis of the internal consistency of the questionnaire responses was performed using cronbach's alpha coefficient (α). This coefficient values the mean correlation between the answers to the questionnaire by analyzing the profile of the answers given by the respondents. The cronbach's alpha calculation procedure is presented in the Supplemental Material. The alpha value obtained was 0.47, setting below the limit of 0.7 which is considered satisfactory (Braun et al., 2021). However, it is worth noting that the value obtained from alpha is considered satisfactory, because the questionnaire has few questions (six questions), and also the questions of the questionnaire were not measuring the same construct or same dimension (one-dimensional), and because of this fact they do not present correlation between the questions, which contributes to a lower alpha value (Bujang et al. 2018; Ekolu and Quainoo, 2019).

The weighting factors of each criterion was calculated using the average ranking (AR). This method is recommended for the analysis of the Likert scale (Soares et al. 2017). The AR considers the weighted average of the answers and the number of respondents. The weighted average considers the observed frequency of each response for each item and the mean value of each response. The AR calculation procedure is presented in the Supplemental Material. The weighting factor of each criterion ranges from 0.00 to 1.00, and when closer to 1.00 the best criterion was evaluated and its importance and influence in the analyses in which it will be used.

2.3.1.3 Ranking of aggregation methods

Based on the defined criteria and their weighting, the LCSA aggregation methods were ranked. For this, all methods were evaluated in the selected criteria considering a numerical scale from 1.00 to 3.00. In general, the scale values represent: value 1.00 the criterion is not met by the method, 2.00 the criterion is partially met by the method and 3.00 the criterion is fully met by the method. For each criterion the scale values are defined in more detail in the Supplemental Material.

The ranking of aggregation methods was performed considering the numerical scale classification score with the weighting weight of each criterion. Multicriteria decision methods (MAVT, TOPSIS, VIKOR and PROMETHEE) were used to determine the ranking of aggregation methods. The multicriteria methods were selected because they are the best known by researchers in the area and because they involve multiple criteria and weighting weights. The best aggregation method based on the evaluated criteria is the one in which the ranking score is higher in MAVT and PROMETHEE, and lower in TOPSIS and VIKOR.

After the application of the multicriteria methods, the aggregation methods were classification by ranking. To determine the final ranking of the aggregation methods, the sum of the ranking position of each method (MAVT, TOPSIS, VIKOR and PROMETHEE) was made, and thus, the best method is the one that resulted in the lowest sum of the ranking positions. For example, consider the aggregation methods "X", "Y" and "Z". Applying the multicriteria methods (MAVT, TOPSIS, VIKOR and PROMETHEE) to the ranking positions of the "X" method were 1, 1, 1 and 3; of the "Y" method were 2, 2, 3, 1, and the "Z" method were 3, 3, 2, 2. The sum of the ranking positions of the methods were in the method "X" of 6, "Y" of 8 and "Z" of 10. Thus, the final ranking classification is method "X" in 1°, method "Y" in 2° and method "Z" in 3°. More information about the calculation procedure can be checked in the Supplementary Material.

2.4 Proposal of a LCSA method

The proposal of a method of aggregation of LCSA was carried out based on the ranking of LCSA aggregation methods. The methods that achieved the highest ranking score were submitted to a more careful analysis of their strengths and weaknesses in relation to the analyzed criteria.

The strengths were compiled to address the shortcomings of the methods, with the proposal to address all the criteria considered as much as possible. Therefore, based on the original premises of the method and the suggested optimizations, an optimized LCSA aggregation method was defined.

In order to validate the proposed method, the method was applied in the case study data of this article, and also in data from other studies, selected according to the presentation of the data in the studies, those that further detailed the data of the results were randomly selected to be used in the validation of the proposed method. Thus, validation was performed considering the standardization method used by the study, as well as the weighting factors.

Another analysis was sensitivity, varying the normalization methods presented in this article and also the weighting weighting weights. The variations in weighting weights considered were: (i) equal weights for all impact categories (i.e. considering the data from the case study in which 11 impact categories are available, the weighting weights are: 1.00/11 = 0.090909091); (ii) equal weights for sustainability classes (i.e. 1.00/3 = 0.333333); (iii) weight of 0.50 for the environmental category and 0.25 for economic and social; (iv) weight 0.50 economic category and 0.25 for environmental and social categories; (v) weight 0.50 social category, 0.25 for economic and environmental categories.

3. Results and Discussion

3.1 Description of methodologies

Initially, an analysis of existing methodologies for aggregating the results of life cycle analyses was performed, as well as the normalization and weighting methods used in the studies. Through the application of the selected methodologies it was possible to identify advantages and disadvantages of each methodology.

A total of 17 different methodologies were identified to aggregate the results of life cycle analyses. These methodologies involve multicriteria analysis methods as well as other methods. While six normalization methods were identified, and 11 different weighting methods were identified in the selected studies. The quantitative distribution of aggregation, standardization and weighting methodologies can be verified in Figure VI – 1.

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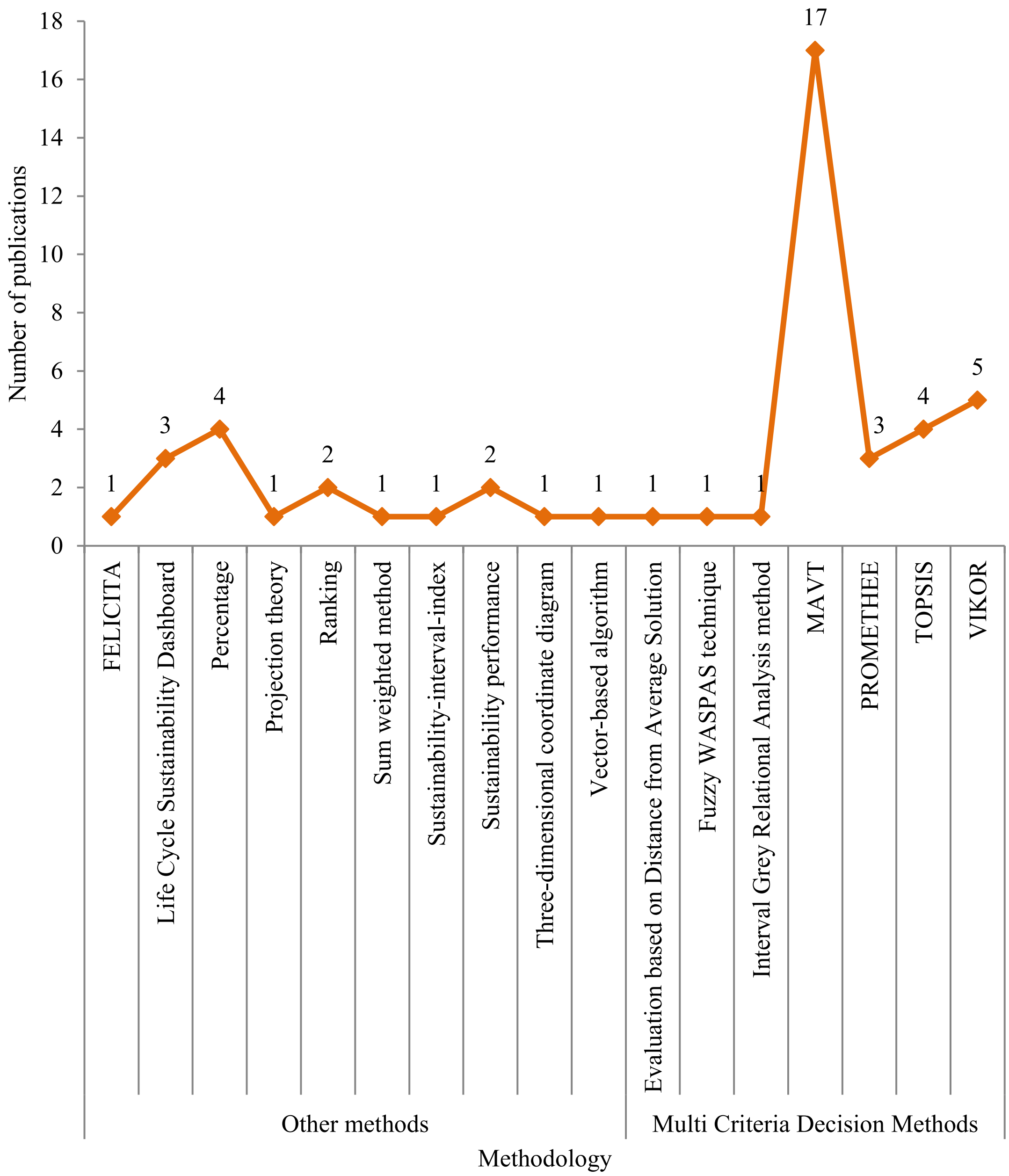
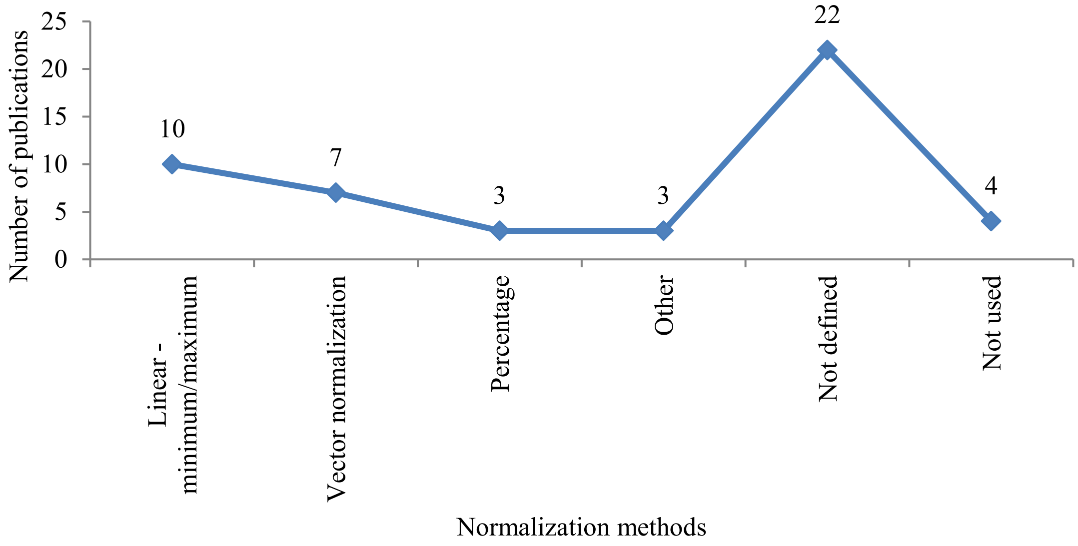
Figure VI - 1: Quantitative aggregation, normalization and weighting methods in LCSA.

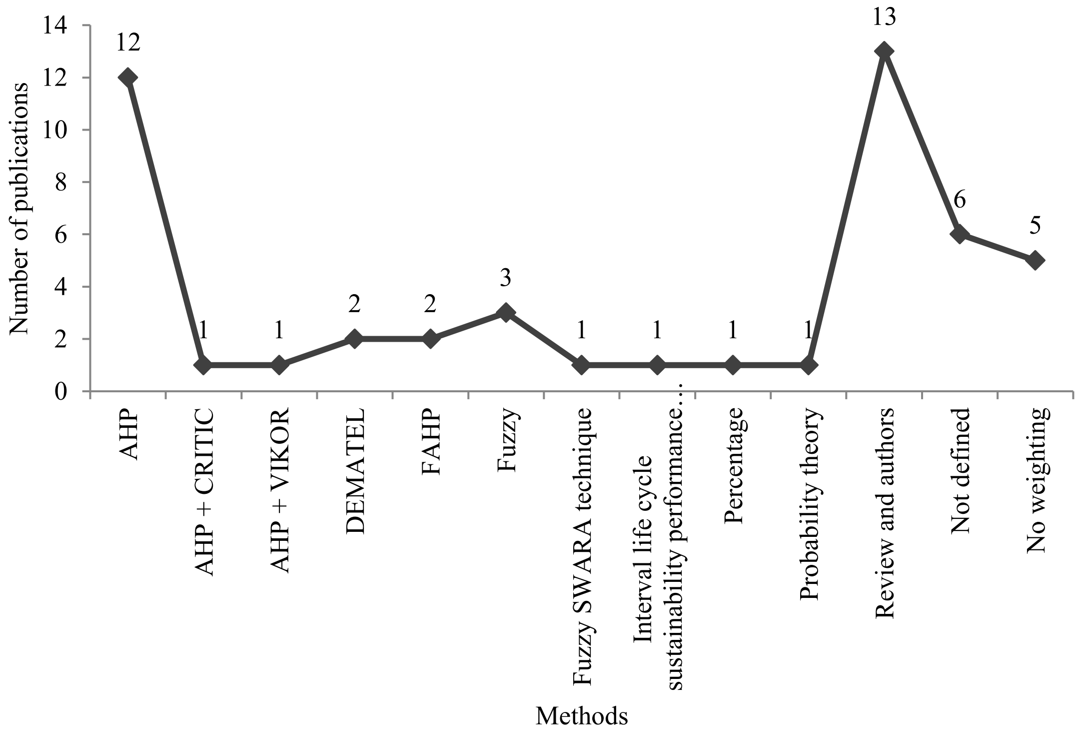
(a)



(b)



(c)



In relation to aggregation methods more than 65.3% of LCSA studies that aggregated the results of life cycle analyses, multicriteria analysis methods were used. Sustainability is a concept that involves multiple criteria, which justifies the majority of use of these methods. However, multicriteria methods can be more complex than other methods, such as ranking and percentage. There is no pattern of methods for LCSA, but it is perceived that the MAVT method is the most used by the authors, corresponding to 34.7% of the studies.

Normalization of the results of life cycle analyses is not an essential step to aggregate the results into a sustainability score, methods such as ranking do not require standardization, and percentage methods use this resource for standardization. However, most aggregation methods require the use of normalization methods, because the results of life cycle analyses are expressed in different units, and to perform an appropriate comparison, these should be normalized in common units.

The most used normalization method was the minimum/maximum linear method, corresponding to 25.0% of the studies, then the vector normalization method corresponds to 17.5%, the percentage method was also used. The methods described as others correspond to a method of division between each environmental and economic aspect (Wang et al., 2017), the normalization method was made by dividing the impact value by factors such as CO2 emissions, number of employment, costs (Aziz, Chevakidagarn and Danteravanich, 2016) and also division by baseline (Tossi et al., 2022). Some studies did not define the standardization method used, while studies with the ranking and sustainability performance method do not use standardization.

Weighting can be considered an important but not essential step in the analysis of life-cycle sustainability. Weighting is a way of representing the opinion of stakeholders and decision makers in relation to what is being evaluated. The use of weighting factors in these cases can be a good strategy to identify the most sustainable solution considering the context of the participants, thus the analysis becomes more robust and representative of that context.

Not using weighting factors, or using equal weighting factors for all impact categories or aspects of sustainability may not result in significant differences in sustainability scores (Visentin et al. 2020). The most used method is the AHP, corresponding to 28.5% of the publications, another highlight is the definition of weights through bibliographic review and also by the authors (for example, using equal weights), corresponding to 26.5%. Some studies did not define the weighting method used, and in some aggregation methods no weighting factors were used.

In the supplementary material, the categorization of the articles presented is presented in detail, highlighting the method of aggregation, standardization and weighting used.

Table VI - 2 presents a general analysis of the methods, containing the description, disadvantageadvantages and studies that used the methodology.

Table VI - 2: Methods of aggregation of sustainability in LCSA, description, advantages and disadvantages.

Method	Description	Advantages	Disadvantages	Reference
FELICITA (Fuzzy Evaluation for Life Cycle Integrated Sustainability Assessment)	The method uses fuzzy logic to determine lifecycle sustainability. Initially, the results of life cycle analyses are normalized. Then defuzzification occurs in the data, using fuzzy relationships to determine the linguistic values corresponding to the classification (bad, average and good). The next step refers to the fuzzy interference process, through the "if then" rules by comparing each impact category with the rules. The number of rules is defined based on the number of categories of environmental, economic and social impact. After the results of the fuzzy interference step are quantified using the data defined in the defuzzification step. This process occurs for each lifecycle analysis, and after for LCSA.	The method is well explained by the authors, and with this facilitates understanding for use in other studies. The use of fuzzy inference is a good alternative to deal with inaccurate and uncertain information in sustainability assessments. The fuzzy inference approach aims to facilitate the process for stakeholders and decision makers who can relate better to verbal "if then" rules than to mathematical expressions that require a more accurate set of values.	The method is more complex, requires many steps which can make practical use as an LCSA methodology difficult. For example, in the fuzzification process stage, linguistic values are assigned to each category of environmental, economic, and social impact. The first classification is defined based on normalized values. After that, an analysis is made based on the theory of combinations, through IF-THEN rules. The amount of impact categories of each lifecycle analysis is an important factor for the amount of rules required in the analysis. For example, an LCA with four impact categories, and considering the three initial linguistic values, has, based on the theory of combinations, for	Kouloumpis and Azapagic (2018)

			the LCA the rule base consists of $3^4 = 81$ rules. In the linguistic values step there is no clarity for the classification of the rules in the result of the if-then analysis. The method used manually results in a lot of complexity, a good alternative is to create a computational program with this methodology, so users would only enter with the values of the results of the life cycle analyses (normalized or not) and the program would perform the entire calculation process, and this would enable the practical use of the methodology.	
Life Cycle Sustainability Dashboard	This method presents the results by means of a graphic representation through a cartogram characterized by a chromatic scale and a classification score. The sustainability performance is displayed through a code of seven	Results in an aggregate sustainability score. It's visual, uses color scales to illustrate sustainability.	The method was the first to be elaborated and used for LCSA, however, only in 2012 the method was used. It is in free software that requires specific operating system requirements to be	Schau, Traverso e Finkbeiner (2012); Traverso et al. (2012a); Traverso et al. (2012b)

	colors ranging from dark red, which represents "critical" conditions, to yellow "average" conditions, to "better" dark green conditions. Each individual performance indicator and topic or the overall index can be highlighted by the arrow position at the top of the panel.		installed, which can make it difficult for many users to use.	
Percentage	The percentage-based method can be used in several ways. Masiela and Pradhan (2021) deteminem a percentage value for each dimension, this value is converted into a scale according to the score weighting system of the authors. After the individual analysis of each aspect of sustainability, the same percentage value reaction is made to determine the sustainability performance index. Padi and Chimphango (2021) sustainability is determined by normalization with the percentage, then the normalized value is multiplied by weighting weight, and	It is a simple method, with a simple calculation process and widely used in day-to-day life. It allows the participation of interested parties through weighting weights, such as the Padi and Chimphango method (2021).	Some methods may not provide for the participation of interested parties through weighting weights.	Masilela and Pradhan (2021): Padi and Chimphango (2021) Tsambe et al. (2021); Al-Yafei et al. (2022)

	finally a sum is made to determine sustainability. Tsambe et al. (2021): the authors propose a methodology for summing the score of each impact category based on a score scale from 1 to 5 and percentage values. The normalization of the results of life cycle analyses is done by converted into contribution percentages, considering the highest values (of environmental, economic and social impacts) as a reference value. After a classification of the percentage results is made according to the scale defined by the authors. The sum of the scale values in each aspect results in another percentage analysis, and finally, the sum of percentages in decimal values is defined as the sustainability index.			
Sustainability performance	This method is based on a position analysis considering as the basis ideal key performance indicators (KPIs) of each aspect of sustainability. The method uses the	There is no need to normalize the results of previous analyses. The method is simple, only requires attention in the correct use of	Setting KPIs values can result in difficulties and even problems using the method. In cases where there is no ideal situation analysis or no	Janjua el al. (2019; 2021)

	likert-5 ponts scale as a basis for calculating position, gap and sustentabilidy performance.	formulas for calculating the score (P). Setting Threshold values can result in some difficulty for the user. This value can be defined for each product according to the results of life cycle analyses, or also based on previous studies, government reports, among others. Sustainability can be classified according to the values of the 5-point likert scale.	participation of stakeholders, KPIs values can be defined considering the results of life cycle analyses, which may benefit a particular product/case study, and not reflecting the actual behavior.	
Projection theory	The aggregate sustainability index of the life cycle is determined based on the sustainability performance matrix of the life cycle and the weights of the criteria for sustainability assessment. Weighting weights are determined through an interval preference relation based goal programming model. This method uses interval values in sustainability aspects and weighting weights. An ideal solution is	It allows the participation of stakeholders by defining weighting weights. It considers the uncertainties through the calculation of the probability matrix. The use of interval numbers to represent the relative preferences between each pair of criteria helps in the ambiguity, inaccuracy and	The method lacks in defining how the intervals of lifecycle analysis results can be determined. However, considering the weighting weight range, you can calculate intervals for each impact category. In the application of the method, the alternative used to define intervals was based on the normalized results of the life cycle, and based on the	Ren (2018a)

	determined, and with this is calculated the projection of each alternative in the ideal solution. A projection probability matrix is determined by comparing each alternative. With this, the sustainability ranking of each alternative is calculated, considering that the higher the value of the sustainability index, the more sustainable the alternative is.	hesitation existing in human judgments.	range of weighting weights presented in Ren et al. (2018a). Thus, the results of the life cycle analyses were multiplied by the values of the weighting weight ing range, thus determining an interval for applying the method.	
Ranking	Score from 1.00 to 3.00 for each sustainability indicator in the environmental, economic and social categories. Score from 1.00 to "x", with "x" being the number of alternatives evaluated. Being the value 1.00 represents the best performance and 3.00 or "x" represents the worst performance. Based on the preliminary results of environmental, economic and social analyses, the scores for the sustainability ranking are defined. It is assumed that all indicators have	Simple and easy methodology to be understood and applied. Based on the results of previous analyses the user classifies each indicator according to the score scale defined. The method is a good alternative of aggregation of results, in order to obtain a sustainability score. There is no need to normalize the results of previous analyses because a	There is no clear criterion for classifying the indicators in the scores, one can use the maximum and minimum values of each indicator, however the classification form could be more detailed. Do not consider weighting factors. However, there is the possibility of including weighting factors, but the authors did not define the calculation method for this, being at the discretion of each user, and it can be a simple sum	Li, Roskilly and Wang (2018); Stamford and Azapagic (2012):

	equal importance, that is, without weighting factor, the score is attributed to each indicator according to performance. All scores are added through a simple sum, so a lower sustainability score indicates better performance and a higher worst performance score.	classification is made on a score scale.	multiplying the weighting factor with the classification score, or perhaps a weighted sum.	
Sustainability-interval-index (SII)	The SII method is based on priority intervals and degree of possibility to determine the most sustainable scenario.	It is a simple method with few steps. It allows the participation of stakeholders in decision-making. The weighting weights of the method are determined using the fuzzy method.	Some difficulties can be found in the practical use of the method in relation to the calculation of the degree of possibility.	Ren et al. (2020)
Three-dimensional coordinate diagram	Sustainability (sustainable value according to the authors' names) is calculated through an equation that relates the results of environmental, economic and social analyses with weighting factors. The sustainable value can be expressed by a three-dimensional graph where the x, y, z axes represent respectively the environmental, economic and social	It is a simple method, the calculation to be performed of sustainability value is simple as well. Considers weighting factors in the calculation. It allows the comparison of results between different studies.	The diagram is an interesting representation of the results of sustainability value, however it can be confusing to be understood. There is no sustainability classification, this is based on the comparison between the evaluated alternatives, and the one that results in the highest	Wang et al. (2017)

	performance of the object of evaluation. The base level means all points where the sustainable value is zero, the most sustainable design alternative is the one that has the longest distance from the base level.		value, that is, the farther away the sustainability value of the base-level of the diagram, the more sustainable the alternative.	
Vector-based algorithm	Sustainability is determined through equations that relate the normalized values of the environmental, economic and social impacts of each alternative with weighting factors. In addition to the sustainability score, the sustainability angle is calculated, which represents deviation from the sustainability performance of an ideal steering process.	The method clearly has the possibility of classifying sustainability according to the value of sustainability magnitude, related to the ideal value according to methodology. The method is simple, the authors demonstrate through practical examples the equations, which facilitates the understanding and application of the method.	There is no sustainability value rating scale. The analysis is done by comparing the value of sustainability and the angle of sustainability.	Xu et al. (2017)
Sum weighted method (SWM)	Sustainability is calculated using a sum that considers the weighting factors with the impact values. The method is similar to Multi-Attribute Value Theory (MAVT), however, in SWM the square root is applied to the values of impacts.	The method is simple, allows the participation of stakeholders in the weighting factors.	There is no sustainability value rating scale. Sustainability is based on the value of the baseline scenario, values close to the baseline scenario are more sustainable.	Tossi et al. (2022)

Interval Grey Relational Analysis method	The Grey Relational Analysis (GRA) is a method for classifying alternatives by calculating the degree of relationship, based on the geometric distance between the reference and the compared sequences. The traditional GRA method is based on sharp numbers, and Ren (2018b) modified the method to consider a decision-making matrix composed of range numbers.	The method allows the participation of stakeholders. It is a simple method, which results in an aggregate sustainability score.	The procedure for calculating the sustainability score is based on intervals, and there is no definition of how to define intervals in studies that there are no intervals. The resulting sustainability score does not have a defined value range, for example, between 0.00 to 1.00. Sustainability is higher the higher the value of grey relational degrees.	Ren (2018b)
Evaluation based on Distance from Average Solution	The traditional Evaluation method based on Distance from Average Solution has been extended by the authors to interval conditions in order to deal with uncertainties. In this method, based on an ideal solution, we seek to verify the distance of each alternative in relation to the ideal situation, and thus the probability is determined by comparing each alternative, finally, the probability matrix is determined and the sustainability score is	The method allows the participation of stakeholders. The method incorporates uncertainties through the use of intervals.	There is no integrated priorities (IP) value classification that represents the sustainability value of each evaluated alternative. The authors only define that the higher the value of IP, the better sustainability, while the lower the value, the worse sustainability is. The method uses intervals, but it is not detailed how the ranges can be defined. The method has several steps, which can make it difficult to use manually.	Ren and Toniolo (2018).

	calculated, called integrated priorities.			
Fuzzy WASPAS (weighted aggregated sum product assessment) technique	Fuzzy WASPAS is based on the weighted product model (WPM) and weighted sum model (WSM) for decision-making development. The aggregation of the results is done based on the multiplicative and summation approach.	The method has a sustainability rating, on a scale of 0.00 to 1.00. The fuzzy method minimizes uncertainty in the data, inconsistencies in evaluations.	The method has several calculation steps. In addition, the method is confusing, with many steps. In the article there is no detail for better practical understanding of the method.	Fetanat et al (2022)
Multi-Attribute Value Theory (MAVT)	The sustainability score is calculated using a weighted sum, which considers weighting weights (calculated by methods such as AHP, VIKOR or determined by users, etc.). The results of life cycle analyses are initially normalized, and after the sum is made considering the weighting weights.	It's a simple method, and the sustainability calculation score as well. The use of weighting weights can express real sustainability according to the opinion of industry experts.	In the MAVT method, the poor performances of some indicators can be compensated by the sufficiently high values of other indicators.	Foolmaun and Ramjeawon (2013); Hossaini et al. (2015); Ren et al. (2015); Atilgan e Azapagic (2016); Aziz, Chevakidagarn and Danteravanich (2016); Akber, Thaheem and Arshad (2017); De Lucca et al. (2018); Ekener et al. (2018); Guo et

				al. (2019); Roinioti and Koroneos (2019); Krysiak and Kluczek (2020); Visentin et al. (2020); Arshad et al. (2021); Figueiredo et al. (2021); Li et al. (2021); Filho et al. (2022); Safarpour et al. (2022); Visentin et al. (2022).
PROMETHEE (Preference Ranking Method for Enrichment Evaluation),	This method does not aggregate the results of life cycle analyses in a sustainability score, it only performs the classification of alternatives, by comparing all the evaluated alternatives. In this method, weights are first assigned to all criteria (indicators) that can be assigned by decision makers, then a preference index is	It is a simple method, there are computer programs that perform the calculations, such as Visual PROMETHEE Business Edition (http://en.promethee-gaia.net/index.html). However, calculations can be done on available tools such as Excel. Allows the	The method does not result in an aggregate sustainability score of the life cycle, it only performs the classification of alternatives. It can be a method alternative for classification, however, an additional calculation process could be done to determine a sustainability score.	Mahbub et al. (2019); Wilken et al. (2020); Wulf et al. (2021)

	calculated for all alternatives considering all criteria and alternatives are classified. In Mahbub et al. (2019) the best path was selected based on the net overtake score. This method is based on the assumption that the higher the score, the better the performance of the alternative (the more sustainable the alternative).	participation of interested parties by considering weighting weights.		
Technique for Order-Preference by Similarity to Ideal Solution (TOPSIS)	The TOPSIS method finds ideal and non-ideal values for the criteria and thus Aa best alternative should have the shortest distance from the positive ideal solution and also the greater distance from the negative ideal solution. In the application of the method, the positive and negative distance of each alternative is calculated, and with these data the closeness coefficients are calculated. The alternatives are classified in descending order based on their proximity coefficients, with the highest value being the best alternative.	The TOPSIS method is a simple method with few steps. The authors clearly define the value limit of closeness coefficients that represents the value of LCSA life cycle sustainability. In this method you can use weighting weights for the impact categories.	Some difficulties may occur in understanding the equations, for example, in the determining the positive-ideal and negative ideal solutions step some categories of impact the higher value is not necessarily positive.	Onat et al. (2016b); Balasbaneh et al. (2020); Maleki et al. (2020); Balasbaneh and Sher (2021)

VIKOR (VIseKriterijumska Optimizacija I Kompromisno Resenje)	The VIKOR method performs the classification and compromise solution through weights. The VIKOR method generates three merit functions that form the basis of the results: "S", representing total uselessness (i.e., total distance from the ideal solution); "R", representing maximum repentance (i.e., worst score); and "Q", an S and R function considering the "commitment strategy" and representing the total score (sustainability score in this case). For all three functions, the range is zero to the unit. The numerical value can be interpreted as the distance of the best possible (ideal) solution; therefore, lower values are considered more preferable.	It is a simple method with few steps. Allows the participation of stakeholders through weighting weights defined by the user or using another method for analysis, such as AHP. It allows an analysis of sustainability according to the conditions described in the article (Zheng et al. 2019).	There is no classification of sustainability, it is made only through the conditions described in the article, comparing the value "Q". A classification could be made with a range of scale values, for example from 0.00 to 1.00, defining sustainability.	Ren et al. (2015); Zheng et al. (2019); Florindo e al. (2020); Aberilla et al. (2021)

3.2 Application of methodologies in the case study

Table VI - 3 presents the results of the sustainability aggregation score of the application of methodologies in the data of the case study by Visentin et al. (2022 - II) and also the ranking of alternatives according to sustainability. It is noteworthy that the application of the methodologies of aggregation of the results followed the steps described by each author, being used the same method of standardization. However, in relation to weighting, equal weighting factors were used, as described in item 2.3. Figure VI - 2 shows the quantification of the sustainability aggregation score of the methods, highlighting the quantification of the classification in less sustainable and more sustainable of each alternative.

In total, 17 different methodologies of aggregation of results were applied, with emphasis on the percentage methodology in which the methodologies identified by the authors differ, and thus, the results of the two forms of the methodologies are obtained. In addition, of all the methods presented, only the Life Cycle Sustainability Dashboard method was not applied because this method is in a program that requires a specific operating system to be installed, not being the case for the availability of the authors.

Table VI - 3: Results of the sustainability aggregation score of the methods and the sustainability ranking.

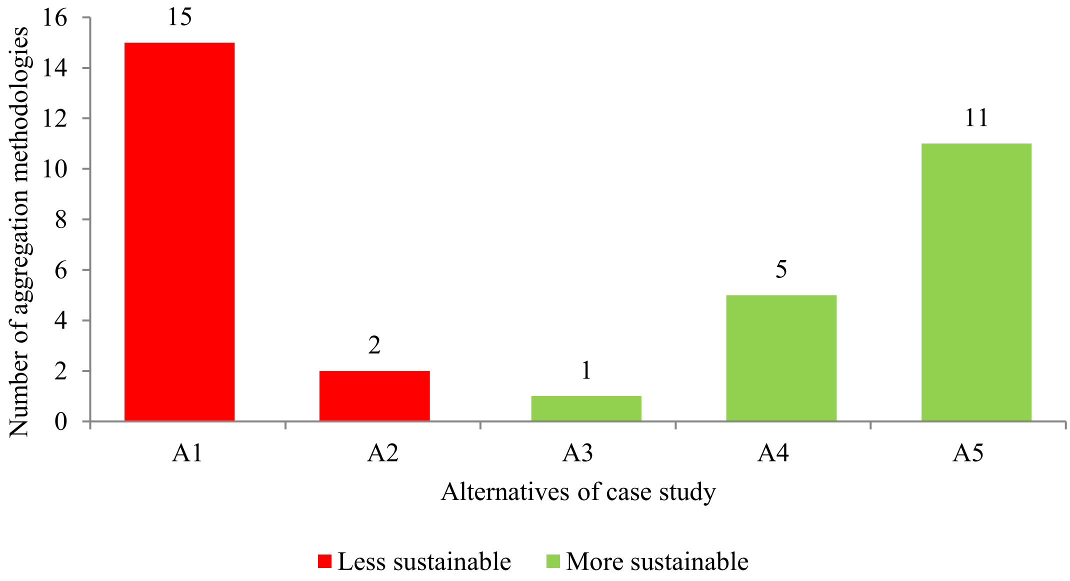
Type	Aggregation methods	Alternatives	Sustainability aggregate score	Ranking
Other methods	FELICITA	A1	0.401	5
		A2	0.669	4
		A3	0.788	2
		A4	0.799	1
		A5	0.787	3
	Percentage	A1	1.520	5
		A2	2.110	4
		A3	2.885	3
		A4	2.905	2
		A5	3.000	1

Type	Aggregation methods	Alternatives	Sustainability aggregate score	Ranking
Other methods	Percentage - Padi and Chimphango (2021)	A1	0.311	4
		A2	0.300	5
		A3	0.769	3
		A4	0.915	1
		A5	0.857	2
	Projection theory	A1	0.100	5
		A2	0.150	4
		A3	0.220	3
		A4	0.230	2
		A5	0.300	1
	Ranking	A1	40.500	5
		A2	34.500	4
		A3	20.500	3
		A4	18.500	2
		A5	14.500	1
	Sum weight method	A1	1.344	5
		A2	1.201	4
		A3	1.086	2
		A4	1.080	1
		A5	1.151	3
	Sustainability-interval-index	A1	0.194	5
		A2	0.211	4
		A3	0.257	2
		A4	0.244	3
		A5	0.292	1
	Sustainability performance	A1	1.589	4
		A2	1.458	5
		A3	3.449	3
		A4	4.523	1
		A5	3.871	2

Type	Aggregation methods	Alternatives	Sustainability aggregate score	Ranking
Other methods	Three-dimensional coordinate diagram	A1	0.819	5
		A2	1.336	4
		A3	19.442	2
		A4	17.897	3
		A5	20.776	1
	Vector-based algorithm	A1	0.277	5
		A2	0.323	4
		A3	0.481	3
		A4	0.494	2
		A5	0.508	1
Multi Criteria Decision Methods	Evaluation based on Distance from Average Solution	A1	0.104	5
		A2	0.156	2
		A3	0.281	1
		A4	0.263	4
		A5	0.196	3
	Fuzzy WASPAS technique	A1	0.451	5
		A2	0.719	4
		A3	0.838	2
		A4	0.849	1
		A5	0.837	3
	Interval Grey Relational Analysis method	A1	6.043	5
		A2	7.532	4
		A3	9.859	3
		A4	9.964	2
		A5	10.903	1
	MAVT	A1	0.424	5
		A2	0.480	4
		A3	0.823	3
		A4	0.846	2
		A5	0.877	1

Type	Aggregation methods	Alternatives	Sustainability aggregate score	Ranking
Multi Criteria Decision Methods	PROMETHEE	A1	-0.406	5
		A2	-0.180	4
		A3	0.170	3
		A4	0.184	2
		A5	0.232	1
	TOPSIS	A1	0.351	5
		A2	0.538	4
		A3	0.926	3
		A4	0.940	2
		A5	0.972	1
	VIKOR	A1	0.573	5
		A2	0.422	4
		A3	0.182	3
		A4	0.082	2
		A5	0.042	1

Figure VI - 2: Quantification of the sustainability ranking of the results of the aggregation score for the ASCV methods in the alternatives of the case study.



Overall, it is perceived that not all methodologies have the same scale of sustainability aggregation score values, methods such as ranking, percentage, Projection theory; Sum weight method; Sustainability-interval-index; Sustainability performance, Three-dimensional coordinate diagram; Vector-based algorithm; Evaluation based on Distance from Average Solution; Interval Grey Relational Analysis method, PROMETHEE. On the other hand, methods (such as FELICITA; Percentage - Padi and Chimphango (2021); Fuzzy WASPAS technique; MAVT, TOPSIS; VIKOR) have a defined range of values, ranging from 0.00 to 1.00.

With the quantification of the ranking of sustainability classification of the alternatives of each method it is possible to verify that in general the least sustainable alternative was A1 being classified accordingly by 88.2% of the methods. Only in two methods did A2 result in the lowest score being classified as less sustainable (Percentage - Padi and Chimphango (2021) and Sustainability performance). The classification of more sustainable varied more in relation to the alternatives, but The A5 was classified as more sustainable by 11 methodologies, corresponding to 64.7%. A4 was classified as more sustainable by 5 methodologies (29.4%) (FELICITA; Percentage - Padi and Chimphango (2021); Sum weight method; Sustainability performance; Fuzzy WASPAS technique). While in just one methodology the A3 was the most sustainable (Evaluation based on Distance from Average Solution).

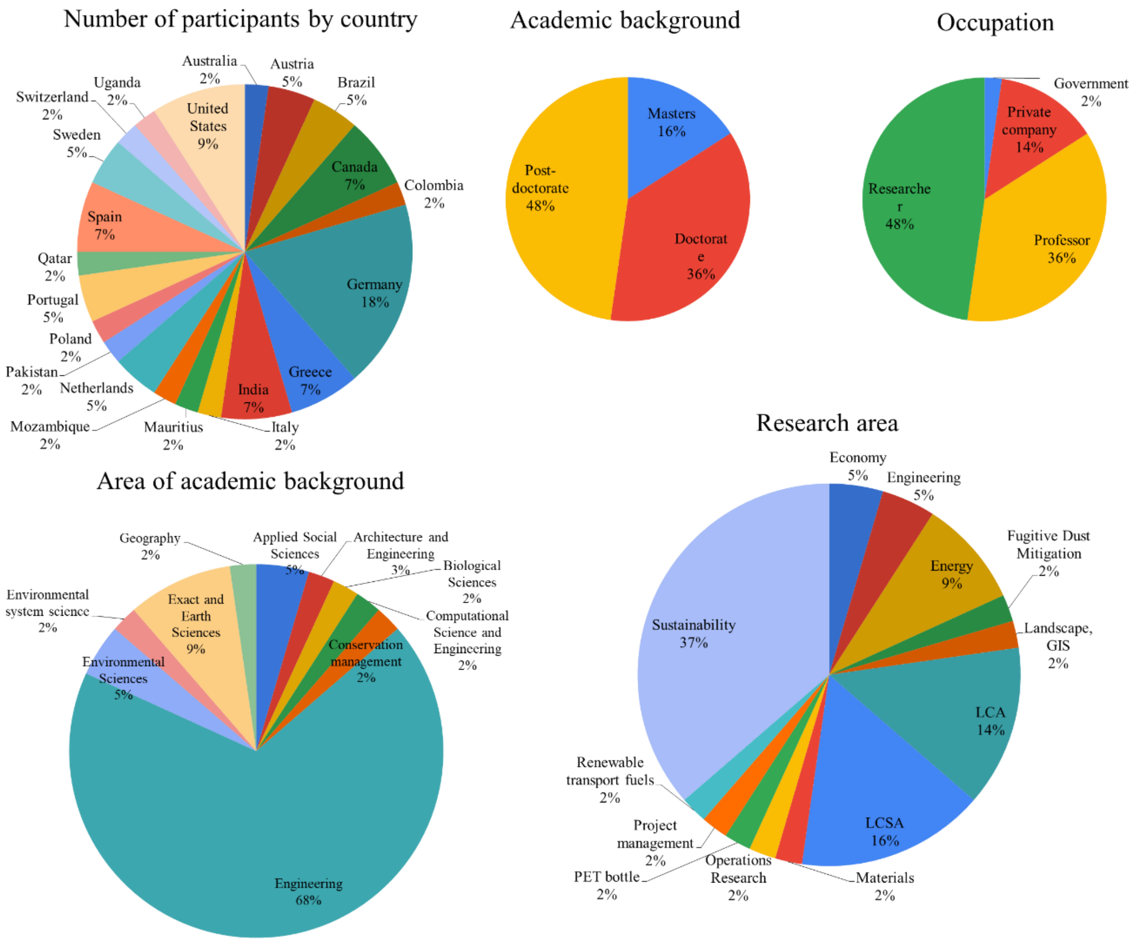
Thus, it is perceived that the methodologies in general indicate that A1 is the least sustainable and the A5 is the most sustainable. However, it is verified how much the sustainability aggregation score can modify according to the methodology used. It is also noteworthy that the different classifications in the ranking do not demonstrate disadvantages in the method, only that according to the equations used and the procedures those alternatives were classified differently. This demonstrates the need to have a universal LCSA method, which can reduce these variations according to different methodologies.

3.3 Analysis of aggregation methods selection criteria

3.3.1 Characterization of participants

The research participants are characterized according to the countries in which they currently reside; training; training area; occupation and research area. Figure VI – 3 presents the characterization in each of these areas.

Figure VI - 3: Characterization of participants.



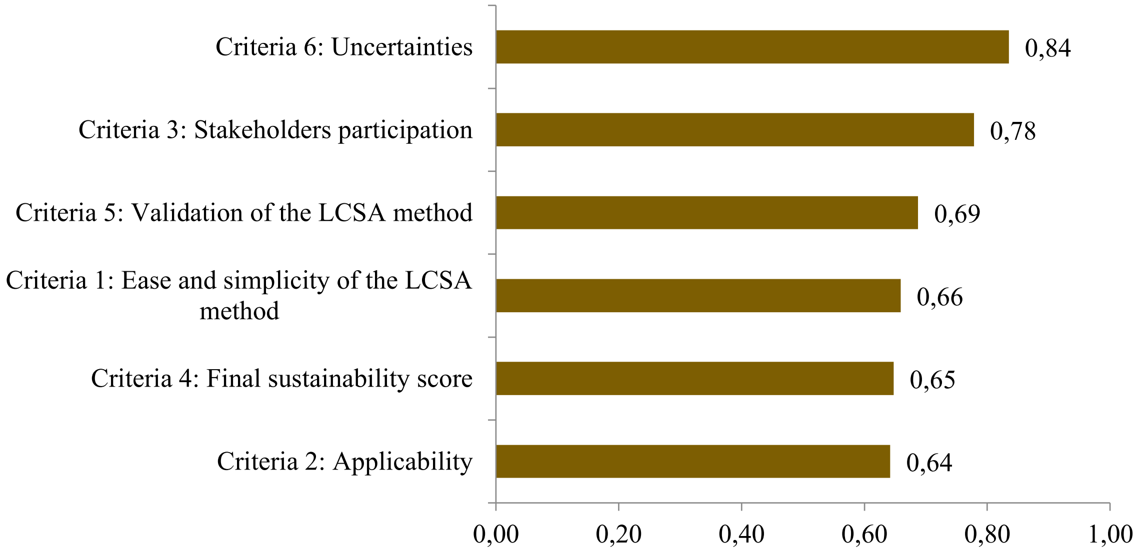
In relation to the country in which the participant currently resides, it is perceived that these are located on all continents. The highlight in relation to the countries is in Germany (8 participants), the United States (4), Canada, Spain, India and Greece (3 participants for each country).

All participants have higher education, with the master's degree being the minimum level (7 participants), the others are doctors (16) and post-doctors (21). In relation to the training area this is multidisciplinary, being the main engineering (30 participants), in addition it has been highlighted for exact and earth sciences (4 participants), applied social sciences and environmental sciences (2 participants each). The occupation of the participants is government, private company, professor and researcher. The research area is varied, with emphasis on sustainability, LCA, LCSA and energy.

3.3.2 Importance and ranking of criteria

Figure VI - 4 presents the list of criteria considered with their importance evaluated by decision-makers using the Likert scale and the average ranking.

Figure VI - 4: Ranking of criteria according to the importance determined by decision-makers.



It is noticed that the criterion best evaluated by the decision-makers was that of uncertainties, that is, the aggregation method should consider the uncertainties in the calculation process. Then there is the participation of stakeholders. The other criteria resulted in similar importance, ranging from 0.69 to 0.64.

Methods that consider uncertainties are typically methods that are based on or that use the fuzzy method, and also intervals. The aggregation methods listed above that consider the uncertainties are: FELICITA; Projection theory; Evaluation based on Distance from Average Solution, Fuzzy WASPAS, Sustainability-interval-index (SII). However, it is noteworthy that the uncertainties in these methods are considered in the stage of definition of weighting factors and not specifically in the aggregation process.

The participation of stakeholders is an interesting mechanism for assessing sustainability considering the context of a given product, local, alternative. However, it is not always possible to consider the participation of stakeholders due to the difficulty of contact, the availability to answer questionnaires, and in some cases even the difficulty in responding consistently.

Some of the research participants suggested the inclusion of criteria, however, the suggested criteria did not necessarily involve LCSA aggregation methods, but rather the entire LCSA calculation process, involving environmental, economic and social analyses. Furthermore, the participants did not assign values to the suggested criteria, which made it difficult to use at this stage. The criterion suggested by two participants was transparency, either in the process of defining weighting weights by specialists, or in general in the LCSA as a whole. Thus, the suggested criteria are presented in the Supplementary Material.

3.3.3 Ranking of aggregation methods

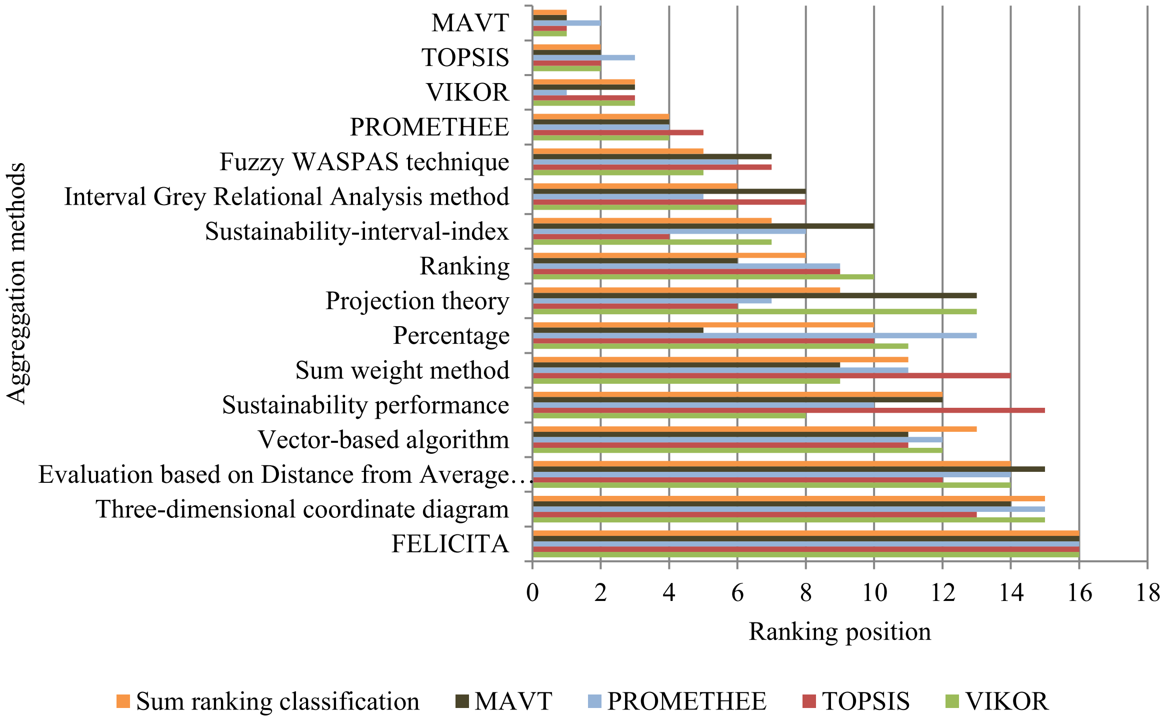
Based on the data on the importance of the criteria and the evaluation of the attendance of each method in the evaluated criteria, the ranking of the aggregation methods selected in this study was performed. Four multicriteria analysis methods were used to determine the ranking (MAVT, TOPSIS, VIKOR and PROMETHEE) and thus be possible to compare the ranking for different calculation procedures. A sum of the ranking positions of each multicriteria method was evaluated to determine the final ranking of the aggregation methods.

Figure VI – 5 shows the ranking of aggregation methods, considering the ranking position by the multicriteria analysis methods evaluated and the final ranking, considering the sum of the ranking positions.

In general, it is noticed that the MAVT method was the best classified by all multicriteria methods evaluated. This method fully meets all criteria except uncertainties, which the method does not consider in the aggregation process. Secondly there is the TOPSIS method, and then vikor. These methods also fully meet most criteria, except for the criterion of uncertainties and ease, which in the VIKOR method have more calculation steps than the MAVT method, for example. The PROMETHEE method was classified in the fourth position, and compared to the methods with better classification, in this method there are more calculation steps than the other previous methods. The four best methods placed are established methods of multicriteria analysis, and with this, the importance of these methods is also verified in the context of LCSA.

The fuzzy WASPAS method was the fifth in the classification, and in this method it is perceived the inclusion of uncertainties, through the weighting method based on fuzzy logic. The method with the worst classification was FELICITA, mainly due to the various steps for calculating the method, which hinders a practical application without a computer program, as previously detailed.

Figure VI - 5: Ranking of classifications of ASCV aggregation methods according to the preference of the criteria defined by the decision makers.



It is noteworthy that the ranking of the determined aggregation methods is based on the criteria determined and weighted by LCSA specialists, as detailed above. Different criteria and weighting weights should modify the ranking of the methods. The objective of this step is not to determine the best aggregation method, but to verify which methods meet the criteria evaluated in order to propose a method of aggregation of LCSA.

3.4 Proposal for a LCSA method

Based on the ranking of the aggregation methods presented in the previous item, an LCSA method was proposed. According to the analysis performed in the previous item, more than 61% of the respondents considered it important or very important to have a universal LCSA method. The proposed method is based on the best classified methods MAVT and TOPSIS. The proposed method has aggregation of two levels, then subindexes and, finally, for a sustainable composite index (CSInd). Figure VI - 6 shows the squeematic figure of the proposed method.

Figure VI - 6: Structure of the proposed method.

Step 01	**Life cycle assessment results** → LCA / LCC / S-LCA → *Impact categories*
Step 02	**Normalization** → *Linear - minimum/maximum* → *Normalized Impact categories (ICN)*
Step 03	**Weighting** → Stakeholder participation - AHP, VIKOR / Definition of equal weights → *Values from 0.00 to 1.00 (w)*
Step 04	**Aggregation level 01 - linear** $Lind = ICN * w$ → *Values from 0.00 to 1.00*
Step 05	**Aggregation level 02 - distance** *5.1 - Determining the positive-ideal and negative ideal solutions.* $\varphi 1 = (\max), (\min) = \{r_1^+, r_2^+, \dots, r_n^+\}$; $\varphi 2 = (\min), (\max) = \{r_1^-, r_2^-, \dots, r_n^-\}$ *5.2 - Calculate distance measures.* $d_{i+} = \sqrt{\sum_{j=1}^{n} (r_{ij} - r_1^+)^2}$ $d_{i-} = \sqrt{\sum_{j=1}^{n} (r_{ij} - r_1^-)^2}$ *5.3 - Calculate Distance Index* $Dind = \frac{d_{i-}}{d_{i-} + d_{i+}}$ → *Values from 0.00 to 1.00*
Step 06	**Composite Sustainability Index (CSInd)** $CSInd = (0.5 * Lind) + (1 - (0.5 * Dind))$ *Values from 0.00 to 1.00*
Step 07	**Sustainability classification** → **CSInd**: 0.00 – 0.20 - Highly unsustainable; 0.21 – 0.40 – Unsustainable; 0.41 – 0.60 – Neutral; 0.61 – 0.80 - Sustainable; 0.81 – 1.00 - Highly Sustainable

Like most LCSA methods, the proposed method, CSInd begins with the results of life cycle analyses (environmental, economic and social). Normalization methods should be used in the first step of the method, these methods can be linear - minimum/maximum normalization, vector normalization, and also percentage normalization. In the next item the sensitivity analysis will check which method is appropriate.

Weighting weights can be defined by the user or also through the participation of stakeholders, for this, weighting methods should be used, such as AHP, VIKOR, Fuzzy. In order to meet the uncertainty criterion (most important criterion evaluated by the specialists, according to item 3.3.2), the fuzzy method is the most appropriate to be used, so this method considers the uncertainties.

The first aggregation of the proposed method is the linear one, which corresponds to the application of the MAVT method. The second aggregation is distance-based, which corresponds to the application of the TOPSIS method. Subindexes are aggregated into a composite sustainability index, according to Equation 1. Finally, the sustainability of the CSInd life cycle is classified according to the classification detailed in Figure VI - 6.

$$CSInd = (0.5 * Lind) + (1 - (0.5 * Dind)) \quad (1)$$

Where:
CSInd: Composite sustainability index (admensional, values 0.00 to 1.00);
Lind: Linear index (admensional, values from 0.00 to 1.00);
Dind: Distance index (admensional, values 0.00 to 1.00).

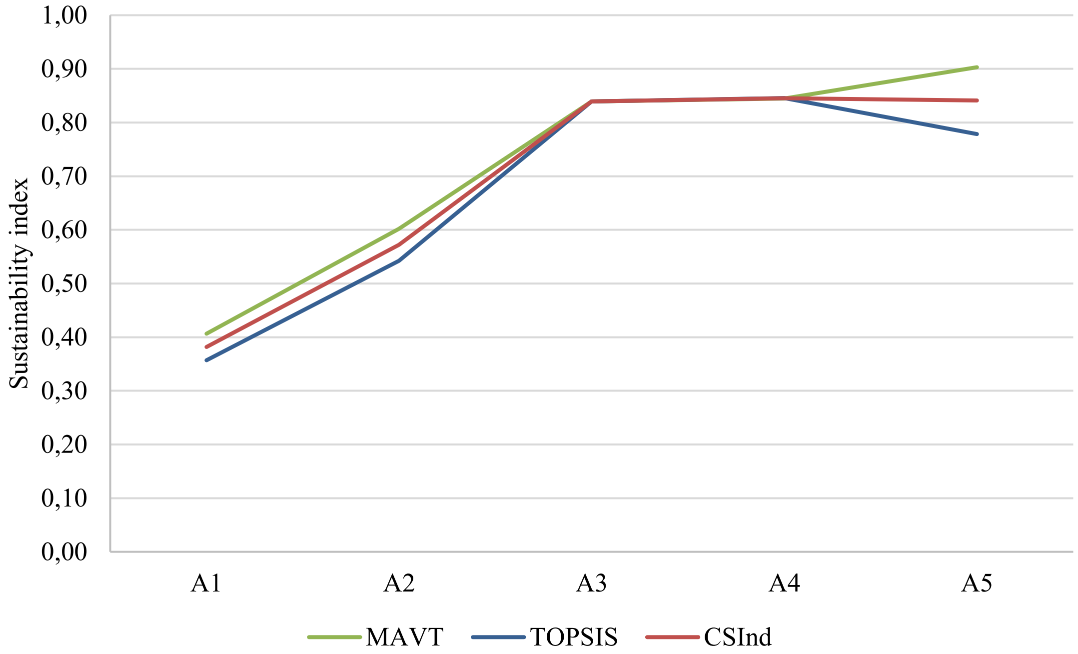
The proposed CSInd aims to compensate the compensability of the MAVT method in which the poor performances of some indicators can be compensated by the sufficiently high values of other indicators. In the TOPSIS method, the measure of similarity with the ideal solution results in that alternatives close to the ideal solution always result in higher scores, while those more distant indexes are lower. Thus, a two-factor aggregation aims to provide a more complete sustainability index, with a more robust result for meeting the limitations of previous methods.

Another factor considering the proposed method is simplicity, CSInd is a simple method to be used, although it has several steps, understanding and calculations are simple. This fact is important because life cycle analyses, LCA, LCC and S-LCA already have a level of complexity. In practice, the LCSA method should be simple, to encourage decision makers to use.

It is noteworthy that, as much as this article aims to propose an LCSA aggregation method, the proposed CSInd method can be applied for any sustainability assessment, not just the life cycle.

Figure VI - 7 shows the application of the proposed method in the case study data presented above, comparing with the application of the MAVT and TOPSIS methods. For this application, the normalization method used was the linear - minimum/maximum and the weighting factor used was the same for all impact categories, i.e., all equal to 1.00/11 = 0.090999. Thus, the most sustainable alternative is the one that results in the highest score of the linear index and the shortest distance to the ideal solution in the distance index, and thus, with higher csind value.

Figure VI - 7: Application of the proposed method, and comparison with the results of the MAVT and TOPSIS method.



It is noticed that the MAVT method results in higher sustainability values, the TOPSIS method resulted in lower sustainability value compared to the MAVT method for all alternatives, especially those in which compensability is verified, such as in A1, A2 and A5. The proposed method, CSInd, resulted in median values compared to the MAVT and TOPSIS indices. Thus, it is perceived that the CSInd will not fully reflect any information about its individual indicators, and thus results in greater accuracy and robustness of sustainability results. The standard deviation of sustainability in comparison with the different methods ranges from 0.0062 to 0.0003, being respectively in A5 and A3 and A4.

Thus, considering the results of the sustainability of the CSInd method, it is perceived that the Alternative A4 is the most sustainable, followed by the alternatives A5 and A3, while A1 is the least sustainable. Regarding the classification of sustainability, the alternatives A3, A4 and A5 are classified as highly sustainable in all methods, except a5 in the TOPSIS method which is classified as sustainable, while A2 is classified as neutral and A1 is classified as unsustainable.

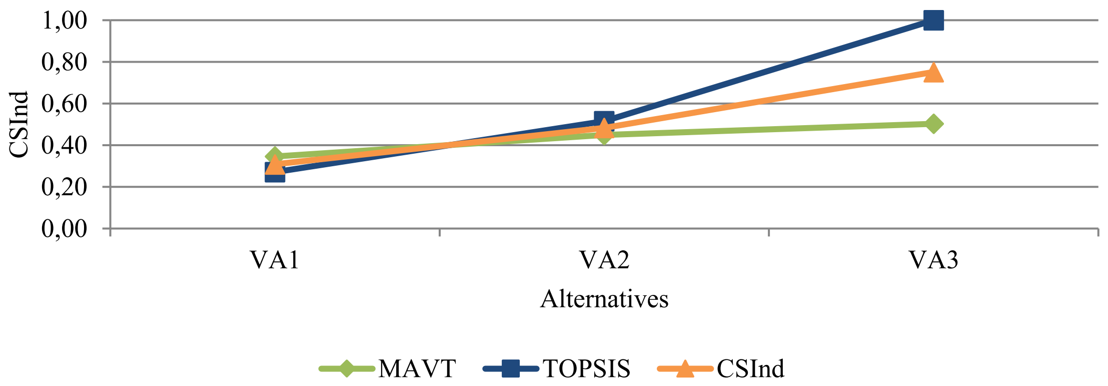
3.4.1 Validation of the proposed method

The proposed CSInd method was validated by applying data from other studies, randomly selected as detailed in item 2.5. Thus, two studies were selected to validate the method: Krysiak and Kluczek (2020) and Atilgan and Azapari (2016). The alternatives of each case study are presented as VA1, VA2, ..., VAn.

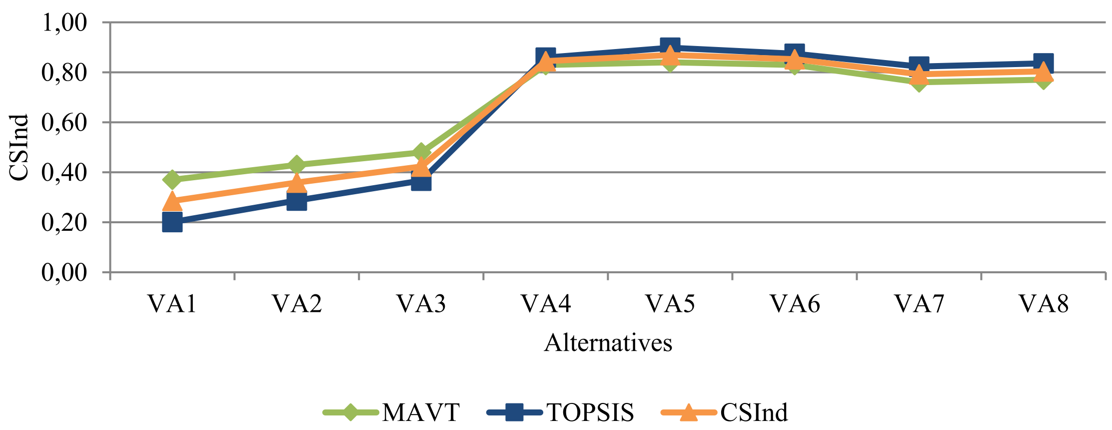
The Krysiak and Kluczek (2020) case study refers to LCSA of chosen photovoltaic modules and three alternatives were considered: monocrystalline silicone crystal (VA1), multicrystalline silicone ingot (VA2), multicrystalline silicone ribbons (VA3). And in the case study Atilgan and Azapari (2016) the LCSA of electricity generation in Turkey was evaluated and eight alternatives were considered: lignite (VA1), hard coal (VA2), gas (VA3), large reservoir (VA4), small reservoir (VA5), run-of-river (VA6), wind (VA7) and geothermal (VA8). Figure VI - 8 presents the results of CSInd validation.

Figure VI - 8: Validation of the CSInd method in other studies. (a) Krysiak and Kluczek (2020). (b) Atilgan and Azapari (2016).

(a)



(b)



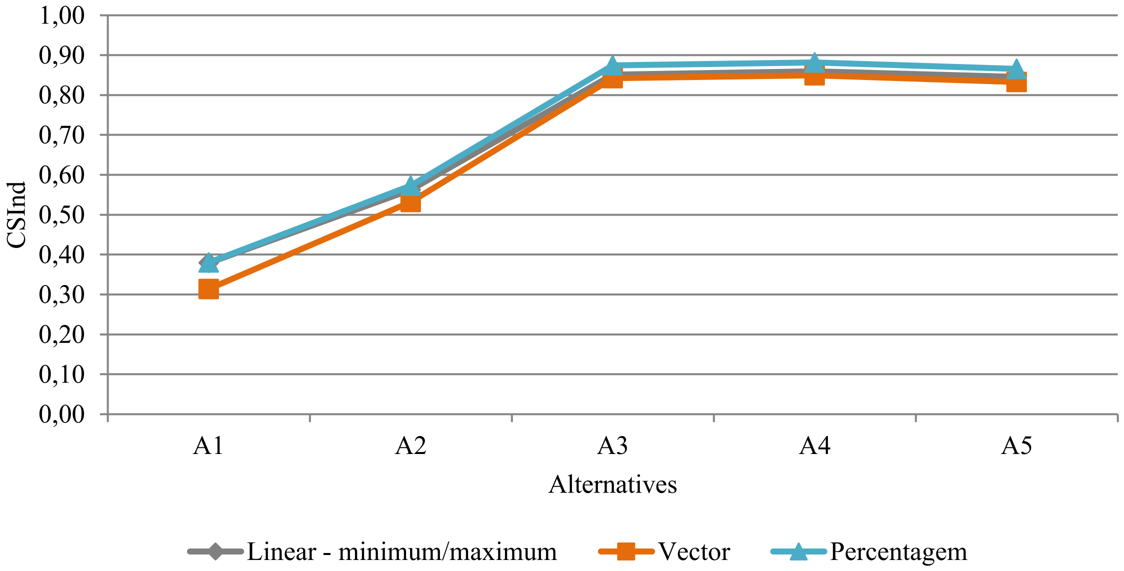
The application of the CSInd method in the selected studies demonstrates behavior similar to that observed in Figure VI - 8, thus validating the method. The results of CSInd result in median values compared to the results of the MAVT and TOPSIS method. And with this, it minimizes the compensability of mavt results and the similarity with the ideal TOPSIS solution. It is noteworthy that the CSInd results are also validated considering the results of the case studies, in which sustainability was higher in the ALTERNATIVE VA3 in Krysiak and Kluczek (2020) and the alternative VA5 in Atilgan and Azapari (2016) in the same way as observed in the authors' studies.

3.4.2 Sensitivity analysis

3.4.2.1 Analysis of standardisation methods

Figure VI - 9 shows the results of the sensitivity analysis varying the normalization methods, the normalization methods were used: linear - minimum / maximum, vector and percentage.

Figure VI - 9: Sensitivity analysis of CSInd in normalization methods.

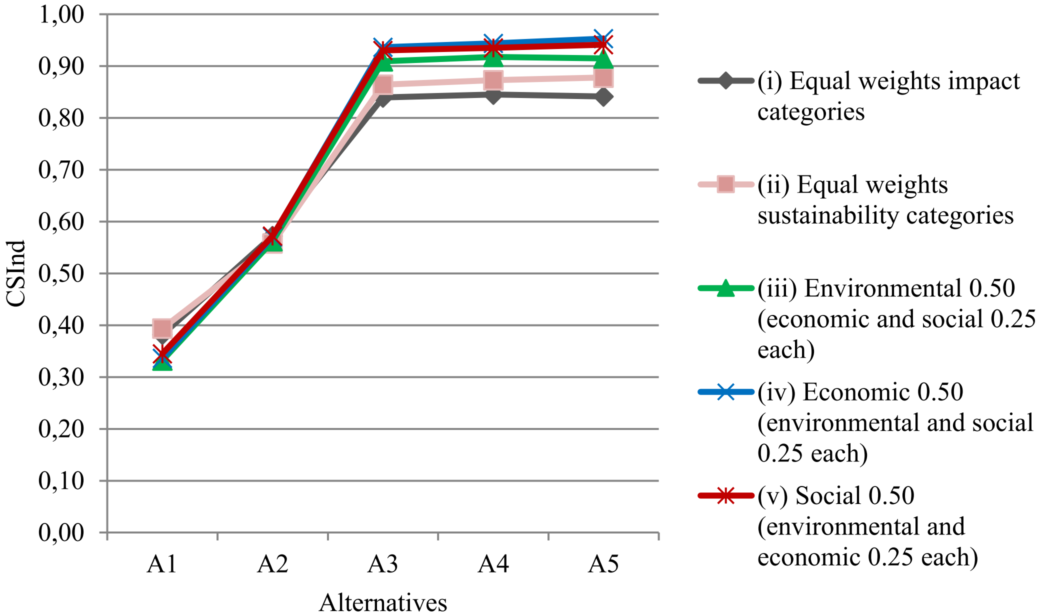


In general, the results are few sensitive to the variation of the normalization method. The standard deviation of the CSInd values comparing the different methods ranged from 0.017 to 0.038. The greatest differences are verified in the vector methods, in which in all case study alternatives it resulted in a lower normalization value. Linear and percentage methods resulted in equal values in all alternatives. Thus, it is perceived that any of these normalization methods can be used in the calculation of CSInd. It is recommended to use the linear method, as it is a simple and easy to understand method.

3.4.2.2 Analysis of weighting factors

The analysis of weighting factors was performed through the variation of weighting weights, considering the following variations: (i) equal weights for all categories of impact; (ii) equal weights for sustainability classes; (iii) weight of 0.50 for the environmental category and 0.25 for economic and social; (iv) weight 0.50 economic category and 0.25 for environmental and social categories; (v) weight 0.50 social category, 0.25 for economic and environmental categories. Figure VI - 10 presents the results of this sensitivity analysis.

Figure VI - 10: Sensitivity analysis varied weighting weights.



The analysis of weighting factors shows that the results are little sensitive to this variation. The largest variations are observed in alternatives A3, A4 and A5, with the standard deviation being 0.042 and 0.046.

In alternatives A3, A4 and A5, it is perceived that the weighting weighting weights with superior preference of the sustainability categories (variations (iii), (iv) and (v)) resulted in the highest CSInd, this fact demonstrates that the superior preference favors the alteratives with better scores in the impact categories, and for this fact the highest scores are verified in these alternatives. In addition, in these scenarios the classification of sustainability becomes highly sustainable in the alternatives A3, A4 and A5.

The use of equal weighting weights (variation (i) and (ii)) results in lower CSInd in alternatives A3, A4 and A5. On the other hand, the alternatives with the worst scores in the impact categories (A1 and A2) the variations in csind are minimal.

The participation of stakeholders is an interesting mechanism for assessing sustainability considering the context of a given product, local, alternative. However, it is not always possible to consider the participation of stakeholders due to the difficulty of contact, the availability to answer questionnaires, and in some cases even the difficulty in responding consistently. For this fact, it is perceived that the non-participation of stakeholders (variations (i) and (ii)) may not significantly affect the results.

4 Conclusion

This study investigated the methods used to aggregate LCSA results into a single sustainability score. Seventheen different methods of aggregating LCSA results were identified, and more than 65% correspond to multicriteria analysis methods, such as MAVT, TOPSIS and VIKOR. While six different normalization methods and 11 weighting methods were identified.

All aggregation methods were applied in data from a case study and there were significant differences in sustainability results both in terms of scoring and also in relation to the ranking of sustainability classification of the case study alternatives.

The proposal of an LCSA method began by analyzing the importance of selection criteria used by decision makers. Thus, the most important criterion of aggregation methods considered by decision makers is uncertainty (0.88), followed by the participation of stakeholders (0.78). Based on the analysis of the methods, criteria and weighting weights defined by decision makers, it was possible to rank the LCSA aggregation methods and identify the best methods, the MAVT and topsis.

Thus, an LCSA aggregation method was proposed. The proposed CSInd method gradually aggregated sustainable development indicators into sustainability sub-indices and, finally, to a composite sustainability index. A sustainability ranking was also proposed, based on the score scale of the results. The proposed method was validated and sensitivity analysis was performed, demonstrating the most appropriate normalization methods and the influence of weighting factors on the results.

Finally, this study contributes to LCSA research by presenting unpublished data from analysis of all LCSA aggregation methods and their application. In addition, this work analyzes the selection criteria of LCSA methods with the participation of important researchers in the area and finally, the proposal of a method that aims to optimize the disadvantages of mavt and topsis methods. Future research should be carried out in order to apply the proposed method in different case and practical studies of LCSA and also in different sustainability analyses. Another perspective of future research is in the consideration of uncertainty in the proposed method.

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Supplementary Material

Articles considered in this study:

Schau, Traverso e Finkbeiner (2012); Stamford, L., Azapagic, A., (2012) Traverso et al. (2012a); Traverso et al. (2012b); Foolmaun e Ramjeawon (2013); Hossaini et al. (2015); Ren et al. (2015); Atilgan e Azapagic (2016); Aziz, Chevakidagarn e Danteravanich (2016); Onat et al. (2016b); Akber, Thaheem e Arshad (2017); Xu et al. (2017); Wang et al. (2017); De Lucca et al. (2018); Ekener et al. (2018); Kouloumpis e Azapagic (2018); Li, Roskilly e Wang (2018); Ren (2018a); Ren (2018b); Ren e Toniolo (2018); Guo et al. (2019); Janjua et al. (2019); Zheng et al. (2019); Mahbub et al. (2019); Roinioti e Koroneos (2019); Aberilla et al. (2020); Balasbaneh et al. (2020); Florindo et al. (2020); Krysiak and Kluczek (2020); Maleki et al. (2020); Ren et al.(2020); Wilken et al. (2020); Arshad et al. (2021); Balasbaneh e sher (2021); Figueiredo et al. (2021); Janjua el al. (2021); Li et al. (2021); Masilelae e Pradhan (2021); Padi, Chimphango (2021); Tsambe et al. (2021); Visentin et al. (2021); Wulf et al. (2021); Yang and Guo (2021); Al-Yafei et al. (2022); Fetanat et al (2022); Filho et al. (2022); Safarpour et al. (2022); Tossi et al. (2022); Visentin et al. (2022).

Table VI - 4: Categorization of the articles presented, highlighting the method of aggregation, standardization and weighting used.

Reference	**Aggregation method**	**Ponderation method**	**Normalization method**
Schau, Traverso and Finkbeiner (2012)	Life Cycle Sustainability Dashboard (LCSD)	Not defined	Not defined
Stamford and Azapagic (2012)	Ranking	No weighting	Not used
Traverso et al. (2012a)	Life Cycle Sustainability Dashboard (LCSD)	Not defined	Not defined
Traverso et al. (2012b)	Life Cycle Sustainability Dashboard (LCSD)	Not defined	Not defined
Foolmaun and Ramjeawon (2013)	MAVT	AHP	Not defined
Hossaini et al. (2015)	MAVT	AHP	Not defined

Ren et al. (2015)	VIKOR	AHP + VIKOR	Not defined
Atilgan and Azapagic (2016)	MAVT	Not defined	Not defined
Aziz, Chevakidagarn and Danteravanich (2016)	MAVT	Review and authors	Other
Onat et al. (2016)	TOPSIS	Fuzzy	Vector normalization
Akber, Thaheem and Arshad (2017)	MAVT	Review and authors	Not defined
Xu et al. (2017)	Three-dimensional coordinate diagram	AHP	Linear - minimum/maximum
Wang et al. (2017)	Three-dimensional coordinate diagram	Review and authors	Other
De Lucca et al. (2018)	MAVT	AHP	Linear - minimum/maximum
Ekener et al. (2018)	MAVT	Sim	Not defined
Kouloumpis e Azapagic (2018)	FELICITA	Not defined	Linear - minimum/maximum
Li, Roskilly and Wang (2018)	Ranking	No weighting	Not used
Ren (2018a)	Projection theory	Interval life cycle sustainability performance matrix	Linear - minimum/maximum
Ren (2018b)	Interval Grey Relational Analysis method	Fuzzy	Linear - minimum/maximum

Ren e Toniolo (2018)	Evaluation based on Distance from Average Solution (EDAS)	DEMATEL	Linear - minimum/maximum
Guo et al. (2019)	MAVT	Review and authors	Not defined
Janjua et al. (2019)	Sustainability performance	Review and authors	Not used
Zheng et al. (2019)	VIKOR	AHP	Vector normalization
Mahbub et al. (2019)	PROMITHEE	Review and authors	Not defined
Roinioti and Koroneos (2019)	MAVT	Review and authors	Not defined
Aberilla et al. (2020)	VIKOR	Review and authors	Not defined
Balasbaneh et al. (2020)	TOPSIS	AHP	Vector normalization
Florindo et al. (2020)	VIKOR	Probability theory	Not defined
Krysiak and Kluczek (2020)	MAVT	AHP	Linear - minimum/maximum
Maleki et al. (2020)	TOPSIS	DEMATEL	Not defined
Ren et al.(2020)	Sustainability-interval-index (SII)	Fuzzy	Linear - minimum/maximum
Wilken et al. (2020)	PROMETHEE	Review and authors	Not defined
Arshad et al. (2021)	MAVT	AHP	Vector normalization
Balasbaneh and Sher (2021)	TOPSIS	AHP	Vector normalization

Figueiredo et al. (2021)	MAVT	FAHP	Not defined
Janjua el al. (2021)	Sustainability performance	Review and authors	Not used
Li et al. (2021)	MAVT	Review and authors	Not defined
Masilelae and Pradhan (2021)	Percentage	Review and authors	Percentage
Padi and Chimphango (2021)	Percentage	Not defined	Linear - minimum/maximum
Tsambe et al. (2021)	Percentage	No weighting	Percentage
Visentin et al. (2021)	MAVT	AHP	Linear - minimum/maximum
Wulf et al. (2021)	PROMETHEE	Review and authors	Not defined
Yang and Guo (2021)	VIKOR	AHP + CRITIC	Linear - minimum/maximum
Al-Yafei et al. (2022)	Percentage	Porcentagem	Porcentagem
Fetanat et al. (2022)	Fuzzy WASPAS technique	fuzzy SWARA technique	Not defined
Fetanat et al. (2022)	Fuzzy WASPAS technique	fuzzy SWARA technique	Not defined
Filho et al. (2022)	MAVT	FAHP	Not defined
Safarpour et al. (2022)	MAVT	AHP	Not defined
Tossi et al. (2022)	sum weighted method	Review and authors	Other
Visentin et al. (2022)	MAVT	AHP	Linear - minimum/maximum

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4. CONCLUSÕES GERAIS

A importância da sustentabilidade nos processos de remediação e também na tomada de decisão foram os principais aspectos avaliados neste estudo. A falta de informações sobre a viabilidade no contexto da sustentabilidade do nFeZ faz com que estudos sejam necessários para auxiliar na tomada de decisão da remediação sustentável. E também, a necessidade de um método de ASCV já vem sendo destacada nos estudos ao longo dos anos. Como forma de contribuir ainda mais para este contexto, foi realizada neste estudo uma análise abrangente e aprofundada da sustentabilidade do ciclo de vida do nFeZ e sua viabilidade de uso na remediação, e também proposto um método otimizado de agregação da ASCV.

A sustentabilidade dos métodos de produção do nFeZ demonstrou que considerando os nove métodos de produção avaliados, o método da síntese verde foi o mais sustentável, enquanto que o método da micro-emulsão foi o menos sustentável. Esta informação é fundamental para que seja realizada a análise do ciclo de vida completo do nFeZ. Além disso, considerando que os nanomateriais podem ser produzidos por diferentes métodos, é importante a divulgação de mais informações referentes aos processos de produção de cada métodos com análises de inventário detalhadas, o que pode contribuir para o aprimoramento da sustentabilidade dos métodos de produção dos nanomateriais, e em especial do nFeZ.

Em relação a sustentabilidade ao ciclo de vida completo do nFeZ, ou seja, da extração dos materiais, produção do nFeZ até o seu uso na remediação importantes contribuições foram determinadas. Para isso, a seleção de diferentes estudos de caso de aplicação do nFeZ na remediação demonstraram que existe diferenças em relação a sustentabilidade do ciclo de vida conforme o uso do nFeZ na remediação. O Estudo de Caso 01 do Brasil foi o menos sustentável, enquanto que o Estudo de Caso 05 dos Estados Unidos foi o mais sustentável. A diferença entre estes dois estudos se dá inicialmente em relação ao nível de saturação do solo, Estudo de Caso 01 é o uso do nFeZ em um solo não saturado, enquanto que no Estudo de Caso 05 em um solo saturado, além disso, os contaminantes e tipo de solo também são diferentes.

Assim, considerando as diferenças entre os estudos de caso, verificou-se que a quantidade de nFeZ utilizada na remediação é o principal fator que afeta a sustentabilidade do ciclo de vida do nFeZ. Aliado a isto, tem-se o nível de saturação do solo, em que foi identificado que solos não saturados requerem uma maior quantidade de nFeZ na remediação do que solos saturados. Outros fatores como tamanho das partículas do solo, permeabilidade e tipo de contaminante também contribuem com a sustentabilidade do uso do nFeZ na remediação.

Através da análise da sustentabilidade do ciclo de vida do uso do nFeZ na remediação dos estudos de caso, verificou-se uma importante lacuna científica a ser preenchida, que relaciona o uso do nFeZ na remediação no Brasil. A viabilidade do uso do nFeZ na remediação demonstrou que a nanoremediação com nFeZ de solos saturados é viável na perspectiva da sustentabilidade, enquanto que a nanoremediação com nFeZ para solos não saturados não é viável na perspectiva da sustentabilidade. A nanoremediação com nFeZ produzido no Brasil pelo método da síntese verde torna a nanoremediação viável na perspectiva da sustentabilidade para solos não saturados. A perspectiva brasileira de uso de nanomateriais na remediação é pequena, ainda há apenas estudos em escala de laboratório, com nenhum registro de aplicação prática em remediação de áreas contaminadas no país.

Por fim, foi feita a proposta de um método de agregação da ASCV. O método proposto tem agregação de dois níveis, depois subíndices e, finalmente, para um índice composto sustentável (CSInd). O CSInd visa compensar as limitações dos principais métodos de agregação da ASCV identificados, e deste modo, fornecendo um índice de sustentabilidade mais completo e com um resultado mais robusto.

Com base em uma análise dos métodos de agregação normalmente utilizado nos estudos, foi possível avaliar estes métodos, e aplicar estes em dados de um estudo de caso, comparando os métodos em termos de aplicação e resultados obtidos. Uma das principais contribuições do estudo, além do método proposto, é na identificação e avaliação de critérios de seleção dos métodos de agregação da ASCV utilizados pelos pesquisadores da área, considerando a sua importância. O método proposto pode ser utilizado tanto na ASCV como também em análises gerais da sustentabilidade.

Contudo, como qualquer desenvolvimento de processo, ajustes, aprimoramentos e novas aplicações são necessárias para alcançar a otimização, a fim de se aproximar cada vez mais de uma metodologia padronizada de ASCV. Além das sugestões já destacadas em cada artigo em particular apresentado neste trabalho, sugere-se que esforços futuros sejam voltados para inserir ao método formas de considerar as incertezas, com adaptações ou inclusão de novos processos.

Propõe-se também como trabalho futuro, o agrupamento, organização e inserção de todas as informações, procedimentos, análises, estruturas e ferramentas desenvolvidas neste estudo em um sistema computacional. O objetivo é de fornecer aos usuários e pesquisadores da área um método útil com interface dinâmica e tangível para a tomada de decisão, e que permite acesso aberto e mais facilitado, rápido e com uma maior interação entre todas as etapas da ASCV.

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