Journal of Cleaner Production 528 (2025) 146697

Contents lists available at ScienceDirect

Journal of Cleaner Production

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

Unlocking nature-based solution potential: Life cycle assessment of groundwater remediation at operating industrial sites

Han Xu [a], Deyi Hou [a,b,*]

[a] School of Environment, Tsinghua University, Beijing, 100084, China
[b] State Key Laboratory of Regional Environment and Sustainability, Beijing, 100084, China

ARTICLE INFO

Keywords:
Benzene contaminated groundwater
Sustainable remediation
Life cycle assessment
Carbon emission
Nature-based solution

ABSTRACT

While life cycle assessment (LCA) has been extensively applied for environmental impact quantification in brownfield remediation, its systematic implementation in guiding groundwater contamination control at operational industrial facilities, where large-scale in-situ remediation is often constrained by ongoing activities, remains less explored. This study seeks to deal with this challenge by conducting a cradle-to-grave LCA of three benzene-contaminated groundwater remediation strategies at an operational industrial site in northeastern China: (1) vertical barriers (VB), (2) pump-and-treat (PT), and (3) a novel nature-based solution (NBS) leveraging phytoremediation with integrated biomass valorization. Results reveal that the baseline NBS scenario (2.63×10^4 kg CO_2-eq, excluding biomass valorization) reduces life cycle greenhouse gas (GHG) emissions by three orders of magnitude compared to traditional VB (1.01×10^7 kg CO_2-eq) and PT (1.44×10^7 kg CO_2-eq) scenarios, showcasing its remarkable sustainability potential. Process-specific optimization pathways, particularly enhanced biomass utilization and carbon storage strategies, further lower GHG emissions to achieve net-positive carbon impacts (-180 kg CO_2-eq/m^3 fiber), thus amplifying green sustainability. The LCA also identified critical process contributors for each of these remediation alternatives and proposed targeted optimization strategies to further minimize environmental burdens across life cycle stages. Overall, by bridging material innovation, adaptive wellfield design, biomass valorization, and life cycle carbon quantification, this study provides scientific support, new perspectives and practical approaches to advance green and sustainable remediation for benzene-contaminated groundwater.

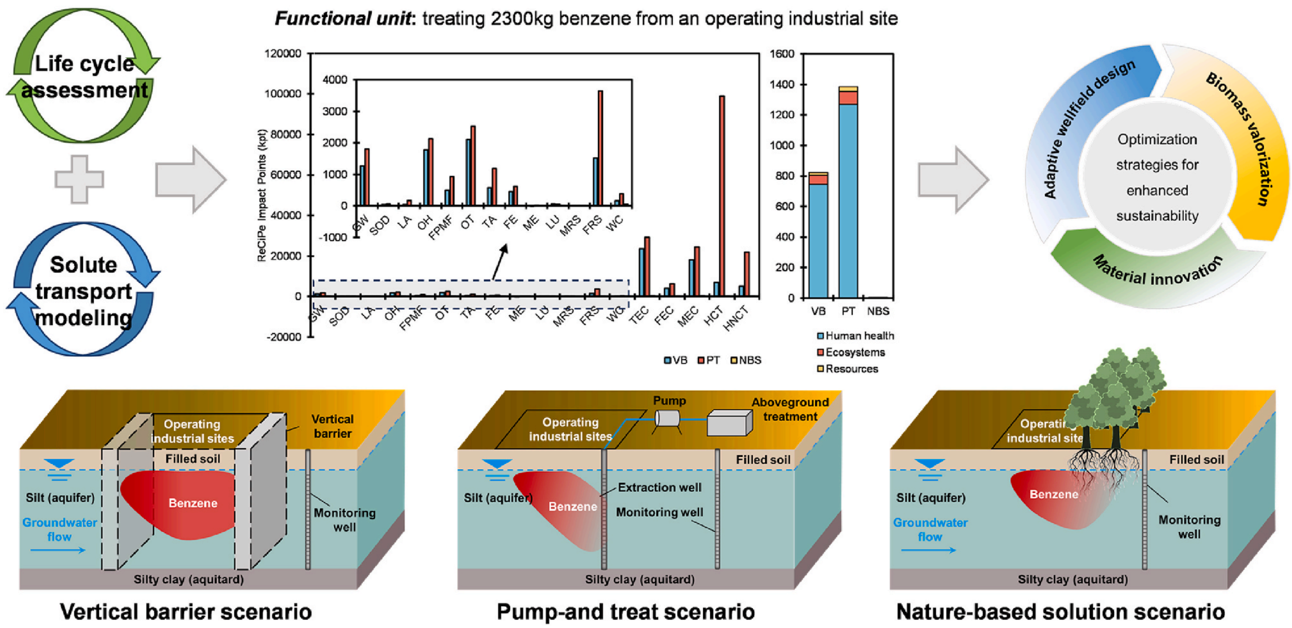
1. Introduction

Although invisible, groundwater accounts for approximately 99 % of the total liquid water on land, providing drinking water sources for billions of people worldwide (Jasechko and Perrone, 2021; Lall et al., 2020; UNESCO, 2022; Wang et al., 2023). In arid and semi-arid regions of northern China, groundwater supplies 65 % of domestic water, 50 % of industrial water, and 33 % of irrigation water (Wang et al., 2023). However, this vital resource faces escalating threats from anthropogenic contamination, driven by rapid industrialization and improper waste management. A 2023 nationwide groundwater quality assessment in China reported that 22.2 % of the 1888 monitored national groundwater quality assessment sites were classified as Class V, indicating the most severe level of contamination (ChinaM.o.E.a.E.o.t.P.s.R.o, 2023). Such contamination poses significant risks to human health, ecosystems, and water security, particularly in regions with high groundwater dependency.

Among groundwater contaminants, benzene is a critical concern. Classified as a light non-aqueous phase liquid (LNAPL), this highly toxic and carcinogenic monoaromatic hydrocarbon (Ahmed et al., 2019; Alshahrani et al., 2022) tends to accumulate above the water table upon release, forming a separate phase that complicates its detection and treatment. In the unsaturated zone, it migrates under gravity until reaching capillary retention, while in the saturated zone, it may persist as trapped residual LNAPL or dissolve into groundwater, sustaining long-lived contaminant plumes (Lari et al., 2019, 2024). Although aerobic and anaerobic biodegradation of benzene is possible, its effectiveness depends on subsurface redox conditions, microbial activity, and soil

* Corresponding author. School of Environment, Tsinghua University, Beijing, 100084, China
E-mail address: houdeyi@tsinghua.edu.cn (D. Hou).

https://doi.org/10.1016/j.jclepro.2025.146697
Received 2 July 2025; Received in revised form 8 September 2025; Accepted 19 September 2025
Available online 30 September 2025



permeability. These behaviors limit natural attenuation in many engineering practices and justify the use of combined physical containment, hydraulic control, and enhanced degradation approaches. Given its health risks, benzene has been classified as a priority contaminant by the United States Environmental Protection Agency (US EPA) and is included in China's initial catalog of 68 priority pollutants in water bodies (USEPA, 2024b; Zhou-Wenmin and Sun-Zongguang, 1991). China, one of the world's largest petrochemical producers, manages extensive petrochemical industrial sites (Zhang et al., 2024). The infiltration of petrochemical pollutants, including benzene and chlorinated hydrocarbons, into soil and groundwater has led to significant environmental degradation, driven by the improper handling and storage of hazardous materials during production and disposal processes (Chen et al., 2022).

Despite the critical need for effective remediation, few studies have systematically evaluated the environmental trade-offs of benzene-contaminated groundwater cleanup. The application of life cycle assessment (LCA) to contaminated site remediation offers a holistic framework for quantifying these trade-offs, balancing remediation benefits against potential environmental costs. However, most existing LCA studies have primarily focused on soil remediation or addressed groundwater contamination involving heavy metal or other organic pollutants (Ellis et al., 2023; Prasannamedha & Kumar, 2020; Van Genuchten et al., 2022; Yang et al., 2023, 2024), offering limited insights into the BTEX (benzene, toluene, ethylbenzene, and xylene) -focused and groundwater-centered remediation, especially for benzene. Besides, previous research has predominantly addressed remediation in brownfield sites or abandoned factories (Alshehri et al., 2023a,b; Hou et al., 2023; Liang et al., 2023; Vincevica-Gaile et al., 2023), neglecting operational industrial enterprises where remediation must coexist with ongoing activities. Such active sites pose distinct technical and management challenges, as remediation strategies must remain compatible with uninterrupted industrial production, limited site accessibility, and stricter regulatory and safety constraints. This necessitates the development and evaluation of remediation solutions that are feasible under complex, real-world operational conditions, contrasting with the relatively flexible implementation settings of brownfield sites. Furthermore, in the context of green and sustainable remediation, while phytoremediation has garnered attention for contaminated site restoration (Alshehri et al., 2023; Alshehri et al., 2023; Hou et al., 2023; O'Connor and Hou, 2020; Wang et al., 2021), its potential for benzene and other BTEX contaminants in groundwater remains underexplored, especially with regard to quantifying its carbon reduction potential and biomass utilization benefits.

To address these gaps, this study employs LCA to evaluate three remediation strategies for benzene-contaminated groundwater at an operational industrial site: (1) vertical barriers (VB), (2) pump-and-treat (PT), and (3) an innovative nature-based solution (NBS) leveraging phytoremediation. The objectives are threefold: (1) to quantify the life cycle environmental impacts of each remediation alternative, (2) to identify key contributors to these impacts and propose optimization measures, and (3) to assess the carbon reduction potential and broaden environmental benefits of NBS, with a particular focus on biomass utilization and carbon storage. By bridging material innovation, adaptive wellfield design, biomass valorization, and life cycle carbon quantification, this study provides critical insights into optimizing remediation strategies that align with low-carbon and sustainable development goals.

2. Materials and methods

2.1. Case study description

The study site is an operating industrial site contaminated by benzene, situated in Shandong Province in Northeastern China. This particular case exemplifies the typical scenario and scale for industrial land contamination resulting from nearby papermaking, thermoelectric and chemical operations. Although the study site covers a modest 18 ha, it serves as a representative and hypothetical model for tens of thousands of hectares of operating industrial land across the province with elevated benzene concentrations. The site of concern in this study maintains an established chemical manufacturing base with operational history exceeding fifteen years. Historical disposal of industrial solid waste, now fully excavated and removed off-site, has led to legacy organic contamination in groundwater, although no continuous source remains at present. Hydrogeological surveys indicate groundwater presence at approximately 5 m below surface level. 20 m depth below the ground surface can be divided into three layers: filled soil, silt, and silty clay. The silty soil layer is the main aquifer with a thickness of about 10 m. The permeability coefficient of the silty clay layer is between

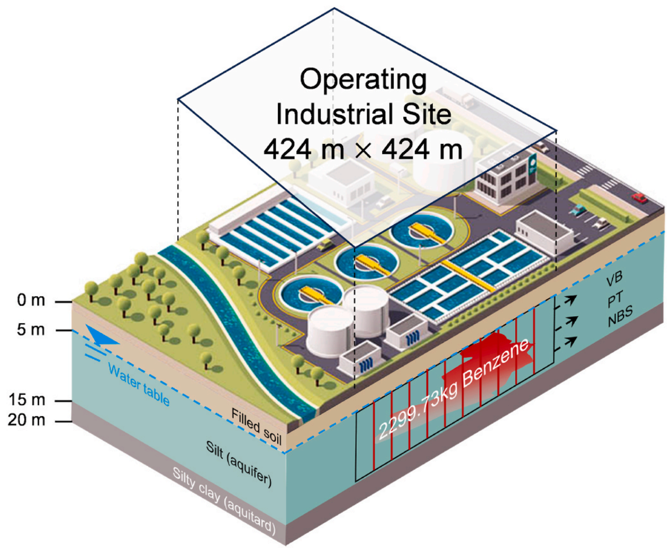


Fig. 1. The conceptual model of the study site.

10^{-6}~10^{-5} cm/s, which is regarded as the aquitard with a thickness of about 5 m. Other hydrogeological parameters include specific yield 0.15, groundwater gradient 0.008, hydraulic conductivity 0.00115 cm/s, and Darcy velocity 0.29 cm/d. The conceptual model of the site is presented as Fig. 1.

A site investigation (2020–2022) identified benzene as the predominant contaminant in groundwater, with concentrations averaging 2300 μg/L, 20-fold exceeding China's Class IV groundwater standard (maximum allowable for industrial use, 120 μg/L) and 230 times higher than Class III drinking water thresholds (10 μg/L) (State Administration for Market Regulation of the People's Republic of China, 2017). Therefore, immediate implementation of risk-based remediation is needed to prevent further aquifer deterioration. Notably, this contamination profile, coupled with the site's active industrial operations, necessitates minimally invasive remediation strategies to mitigate carcinogenic risks (USEPA, 2024a) allow for maintaining ongoing production.

2.2. Remediation scenarios modeling

2.2.1. Conceptual model and technical design

Due to the ongoing industrial production activities of the operational enterprise, large-scale excavation is not feasible for the site. Consequently, based on the specific site conditions, the following three hypothetical scenario models are constructed, aiming to explore eco-friendly remediation tailored to this site and provide a reference for similar cases of benzene-contaminated groundwater. The specific design details of the remediation layout are presented in Fig. 2.

(1) **VB:** Utilizing the naturally occurring weak aquitards such as the underground silty clay layers as a natural barrier, a vertical barrier system is constructed vertically from the surface down to and beyond the natural barrier layer, thereby preventing the migration of benzene contaminants. The filling materials used in the construction of the barrier in this study are cement and bentonite, both of which are widely recognized as standard materials for constructing VB due to their effectiveness in creating impermeable walls (Cheng et al., 2022; Flessati et al., 2023; Gahlot et al., 2022; Sun et al., 2022). To ensure effectiveness, the barrier wall is designed to be approximately 16 m deep, with a wall thickness of 850 mm and a total length spanning approximately 1700 m around the site perimeter. Further key technical parameters are outlined in Table 1, and additional detailed parameters and calculations are shown in Section 1-3 of Supplementary Information (SI).

(2) **PT:** As a widely employed groundwater contamination remediation technology, PT demonstrates excellent applicability in treating BTEX (Ministry of Ecology and Environment, P.s.R.o.C., 2022). Given that the primary aquifer in the study area comprises moderately permeable silty pore media, it is suitable for the application of PT technology. Aiming to significantly reduce contaminant levels and halt the spread of the contaminant plume, an array of 7 extraction wells is situated along the plume's downgradient edge, each with a total depth of 15 m and screened between 5 and 14 m to match the targeted aquifer zone. Key technical parameters are presented in Table 1, and additional detailed parameters and calculations are shown in Section 1-3 of SI.

(3) **NBS:** We employ a phytoremediation strategy by planting 1115 poplar trees within the contaminant plume, specifically near its downgradient edges, at a spacing of 4.8 m by 4.8 m to create a dense and effective hydraulic control and treatment zone. This layout ensures sufficient root zone development (Hong et al., 2001; O'Connor and Hou, 2020; Quinn et al., 2001) and is functionally analogous to an array of extraction wells, acting as "green extraction wells" that form a natural hydraulic barrier

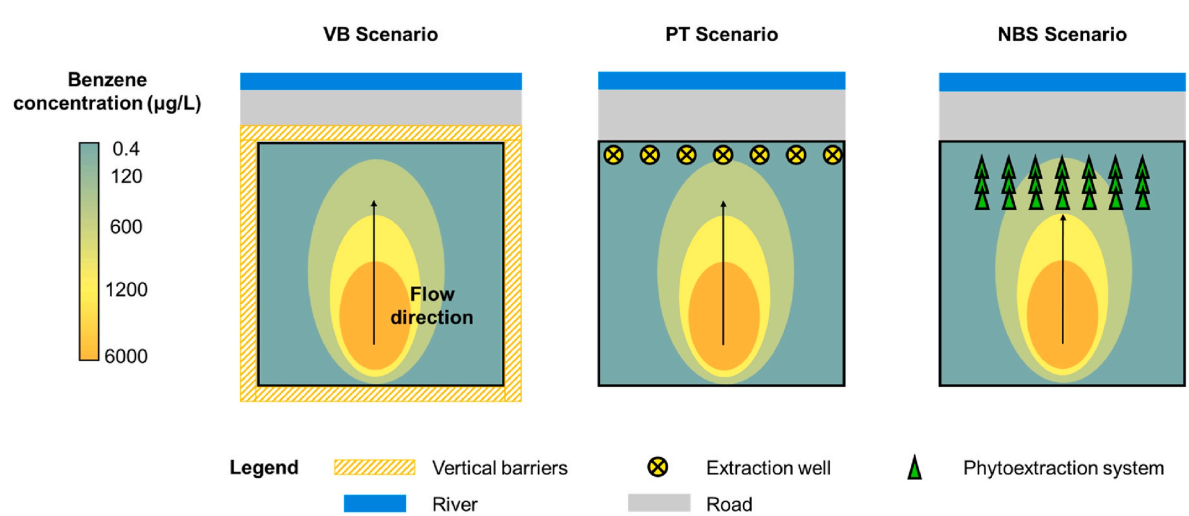


Fig. 2. Plan view illustrations of deployment layouts for three scenarios. Note: The number of wells and plants shown in the figure is just illustrative and does not represent the actual quantity at the site.

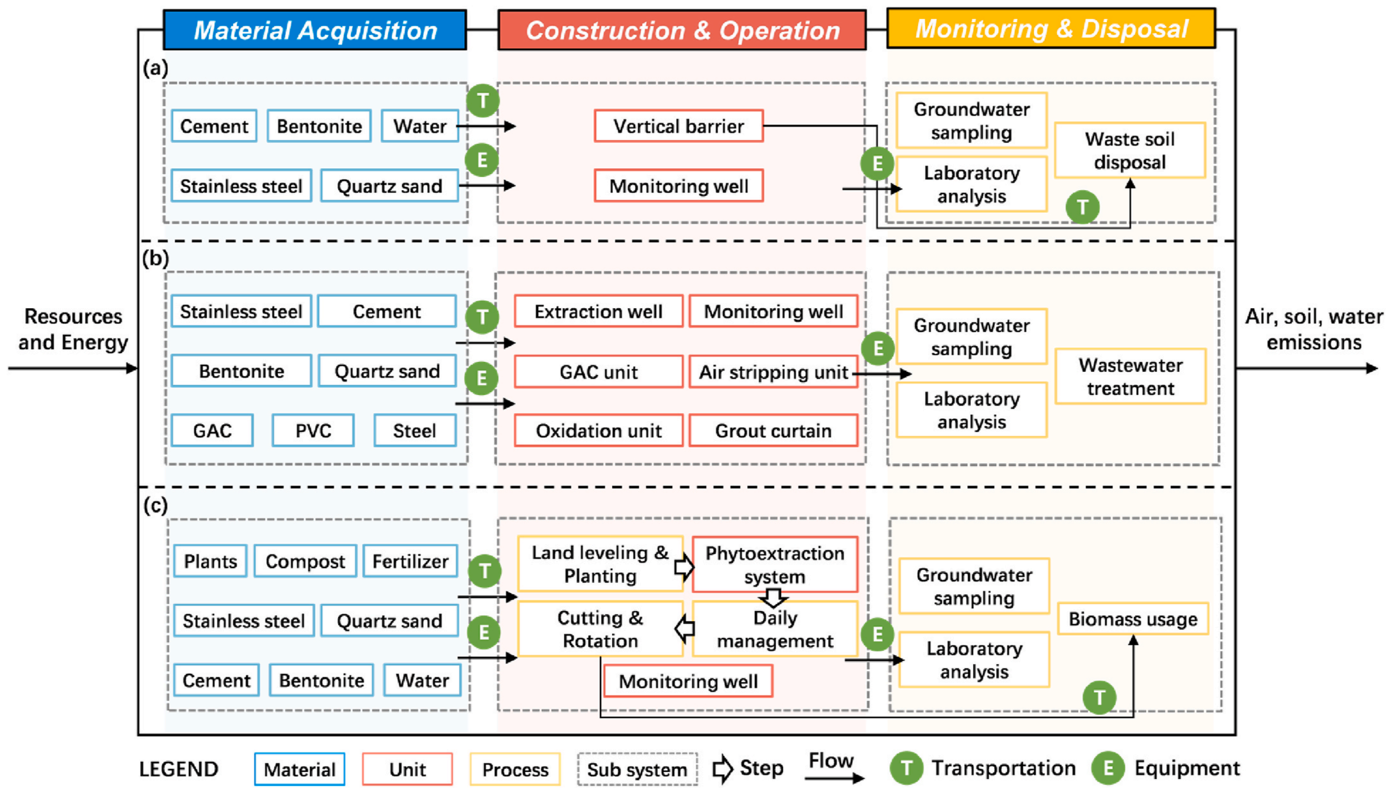


Fig. 3. Remediation system boundaries: (a) VB; (b) PT; (c) NBS. GAC: granular activated carbon; PVC: polyvinyl chloride.

(Aghili and Golzary, 2023; Danielescu et al., 2020; Jin et al., 2021; O'Connor and Hou, 2020; Wang et al., 2019) that reduces contaminant dispersion while simultaneously providing in-situ treatment. The trees collectively establish a cone of depression primarily through phytoextraction, supplemented by phytovolatilization and phytodegradation, enabling passive plume containment. Poplar trees (*Populus 107* in this study) are particularly well-suited for this purpose due to their deep root systems that effectively access groundwater, high biomass production that supports sustained aromatic hydrocarbons uptake, and rapid growth combined with resilience (Ranjan, 2021; Simmer and Schnoor, 2022), which minimizes maintenance requirements and significantly reduces long-term remediation costs. Compared to conventional PT systems, the hydraulic gradient induced by poplar roots is passive and localized but sufficient for controlling plume spread in shallow unconfined aquifers. Meanwhile, this phytoremediation configuration eliminates the need for continuous energy input and aboveground treatment, aligning with low-carbon and nature-based remediation objectives. Key technical parameters are presented in Table 1, and additional detailed parameters and calculations are shown in Section 1-3 of SI.

2.2.2. Numerical modeling of solute transport

To establish the temporal boundary for the LCA, solute transport modeling of benzene migration in groundwater was performed using the MODFLOW and MT3D modules in the Groundwater Modeling System (GMS) software. Hydrogeological parameters were derived from site-specific geotechnical surveys, in-situ testing, and corroborated with literature-reported values under comparable hydrogeological conditions. The modeling results indicated that PT and NBS scenarios required equivalent remediation durations of approximately 30 years (Figs. S2 and S4), which was subsequently adopted as the unified LCA timeframe across all scenarios for consistent comparison, consistent with the documented service life of cement-bentonite barriers in both practice and literature (typically decades) (Cao et al., 2021a,b; Joshi et al., 2010; USEPA, 1998; Zhang et al., 2024). Detailed model parameters, calibration steps, and simulation results are provided in Section 1.3 of SI.

2.3. Life cycle analysis

This LCA study follows the guidelines of ISO 14040 and ISO 14044 (ISO, 2006a, 2006b), employing a four-phase framework: goal and scope setting, inventory analysis, impact assessment and interpretation.

2.3.1. Goal and scope

The goal of the LCA is to evaluate and compare the life cycle environmental impacts of three groundwater remediation scenarios (VB, PT and NBS) for benzene contamination at an operational industrial site.

The spatial boundary is the 424 m × 424 m contaminated site. The temporal boundary is a 30-year service period for all scenarios, capturing both short-term implementation impacts and long-term maintenance. The functional unit is defined as reducing groundwater benzene concentrations below 120 μg/L (2299.73 kg benzene, details see Section 1 of SI) and preventing its migration beyond the site boundary to protect sensitive receptors over a 30-year period.

The LCA system boundary encompasses a comprehensive cradle-to-grave scope, considering multiple sub-systems of modeled scenarios, such as raw material and energy acquisition, system construction and operation, transportation, monitoring, and waste disposal (Fig. 3). Certain minor consumables, such as personal protective equipment (e.g., gloves) and office-related supplies (e.g., paper), are excluded, as they as their life cycle contributions are negligible and do not significantly affect the comparative impact across different scenarios (Hou et al., 2014).

2.3.2. Life cycle inventory (LCI)

Primary data sources for remediation technologies were obtained through multiple channels, including field investigation, scientific publications, and consultations with industry experts, contractors, and

Table 1
Key technical parameters of three remediation alternatives.

Scenario	Parameters	Value
General	Initial benzene concentration	2300 μg/L
	Source zone area	424 m × 424 m
	Aquifer depth	−5 m ~ - 15 m
	Timeframe for the LCA	30 years
VB	Length × Thickness × Depth	424 m × 850 mm × 16 m
	Amount	4
	Cement incorporation ratio	30 %
	Water-cement ratio	1.5
PT	Well depth	15 m
	Inside diameter	213 mm
	Outside diameter	219 mm
	Amount	7
NBS	Plant type	Poplars
	Planting density	4.8 m × 4.8 m
	Amount	1115

equipment vendors. Detailed LCI, including calculation methods, project-specific measurements, and literature-derived inputs, are documented in Section 3 in the SI (Tables S7–S22), where each remediation scenario (VB, PT, and NBS) is systematically structured into subsections covering material inputs, equipment inputs, transportation, and energy consumption. Background system inventory data (Table S23), covering operations from upstream to downstream processes, are derived from the Ecoinvent v3.5 database (Wernet et al., 2016). The electricity consumption for on-site operations was assumed using the average Chinese electricity grid mix, while most other processes lacking China-specific inventory data were estimated based on the global average values. A condensed version of LCI for three scenarios is presented in Table 2, normalized to the functional unit of treating 2299.73 kg benzene in the aquifer of the operational industrial site.

2.3.3. Life cycle impact assessment (LCIA) method

The environmental impact assessment in this study was conducted using SimaPro 8.0 LCA software (PReConsultants, 2014), employing the ReCiPe 2016 methodology at both midpoint and endpoint levels, hierarchist version (Huijbregts et al., 2020). This assessment framework incorporates USES-LCA (Van Zelm et al., 2009) for modeling substance transport, environmental exposure, and ecological effects.

The ReCiPe methodology applies a dual-level approach, comprising 18 midpoint impact categories and three aggregated endpoint damage categories: ecosystem quality, human health, and resource availability. For analytical consistency, this research employs the default ReCiPe endpoint method to aggregate results across these categories into single final scores, thereby enhancing interpretability for conclusion formulation. However, acknowledging the inherent methodological uncertainties associated with endpoint evaluations (Hauschild, 2005), the investigation simultaneously implements the ReCiPe midpoint approach to provide comprehensive, mutually reinforcing analytical perspectives.

2.3.4. Sensitivity analysis

A sensitivity analysis was performed to assess how parameter variations influence the outcome reliability. The selected sensitivity parameters comprised barrier filling material dosage, treatment reagent quantity, and transport distances. These variables were prioritized based on their dominant contributions to environmental impacts, as identified through a contribution analysis of the LCI results (see Section 3.2). Rather than simulating all variables, we focused the sensitivity analysis on those with the greatest influence on key impact categories to ensure methodological relevance and computational feasibility. This focused analysis scope excluded non-critical parameters to maintain methodological rigor while ensuring computational tractability.

2.4. Evidence base and parameterization for optimization strategies

We propose optimization strategies using a hybrid approach that combines (1) literature-informed parameterization, (2) site-specific transport modeling, and (3) system boundary-extension of downstream biomass utilization. The present subsection summarizes the core assumptions. Detailed equations, inclusion criteria, and raw data are provided in Section 4 in SI.

VB: We compiled 17 barrier projects over the past five years to parameterize the trade-off space among hydraulic performance, carbon intensity, and cost (SI, Section 4.1).

PT: We compared 4 alternative wellfield designs using the calibrated MT3DMS model to optimize spatial layouts and pumping rates (SI Section 4.2).

NBS: We synthesized 13 case studies to LCA framework by extending the system boundary to include biomass utilization and long-term carbon storage (SI Section 4.3).

3. Results and discussion

3.1. Overall impacts and uncertainty

The life cycle environmental impacts, presented in characterized and normalized formats within the SI (Table S27), were further analyzed using the ReCiPe 2016 methodology. Normalized results, expressed in person equivalents (PE), are illustrated in Fig. 4, encompassing both midpoint (18 impact categories) and endpoint (3 damage categories) indicators. A higher ReCiPe single score reflects greater environmental burdens, with endpoint impacts dominated by human health damage (contributing 85–90 % across scenarios), primarily driven by global warming, human toxicity, and fine particulate matter formation. This underscores the critical need to prioritize health-centric remediation strategies.

Across all three damage categories (human health, ecosystem damage, and resource depletion), PT (1384.88 PE) exhibited the highest impacts, followed by VB (821.99 PE), while NBS (3.70 PE) consistently demonstrated minimal burdens. Correspondingly, greenhouse gas (GHG) emissions reached 14393 tons CO_2-eq and 10083 tons CO_2-eq in PT and VB, respectively, whereas NBS achieved a carbon footprint of 26 tons CO_2-eq, a reduction exceeding 99 % compared to conventional methods. This large disparity reflects the contrasting material and energy profiles of the systems. PT and VB depend on carbon-intensive materials (e.g., cement, steel, etc.). And in the case of PT, continuous energy input for pumping and treatment, whereas NBS uses low-impact biomass and functions passively. Furthermore, the poplar-based NBS provides additional carbon sequestration benefits, contributing to its near-net-zero footprint. These findings underscore the decarbonization potential of NBS in site remediation, which not only offsets climate-related human health impacts, but also contributes to ecosystem protection by improving air quality and reducing acidifying emissions.

While ex-situ excavation with horizontal barriers remains prevalent for contaminated site remediation (Feng et al., 2020; Lemming et al., 2012; Li et al., 2024), this study's operational constraints, prohibiting large-scale excavation, necessitated perimeter-focused interventions. This limitation significantly contributed to the elevated carbon emissions reported in our analysis, highlighting the pivotal role of layout of barriers in the assessment. Ding et al.'s work offers a comparative evaluation of the life cycle impacts of a Biochar Permeable Adsorptive Barrier (BPAB) and PT methods (Ding et al., 2022), which outperform VB and PT in this study. Ding et al. reported 1860.22 kg CO_2-eq for PT systems treating 1 kg VOC contaminant, a 70 % reduction compared to our findings (6261.60 kg CO_2-eq/kg). This discrepancy arises from fundamental design divergences: their PT system emphasized source-zone containment with limited pumping, whereas our scenario required expansive plume control, significantly amplifying electricity and material demands. Crucially, both studies employed similar

Table 2
Life cycle inventory of three remediation scenarios.

Stages and items	Remediation scenario								
	VB			PT			NBS		
	Amount	Unit	Source	Amount	Unit	Source	Amount	Unit	Source
Material consumption									
Construction									
Cement	8698.86	ton	Tables S5, S7, S8	2.54	ton	Tables S5, S12, S13	0.82	ton	Tables S5 and S19
Water	13047.06	ton	Tables S7 and S8	–			1498.50	ton	Tables S17 and S19
Bentonite	7253.32	ton	Tables S5, S7, S8	15.12	ton	Tables S5, S12, S13	4.96	ton	Tables S5 and S19
Sand	8.12	ton	Tables S5 and S8	24.73	ton	Tables S5, S12, S13	8.12	ton	Tables S5 and S19
Steel	1.27	ton	Tables S5 and S8	3.22	ton	Tables S5, S12, S13	1.27	ton	Tables S5 and S19
Plants	–			–			1115	p	Tables S17 and S19
Compost	–			–			33.45	ton	Tables S17, S18, S19
Fertilizer	–			–			0.54	ton	Tables S17, S18, S19
Sampling and analysis									
Methanol	1.74	ton	Tables S6 and S8	1.74	ton	Tables S6 and S13	1.74	ton	Tables S6 and S19
Ascorbic acid	0.01	ton	Tables S6 and S8	0.01	ton	Tables S6 and S13	0.01	ton	Tables S6 and S19
Hydrochloric acid	0.05	ton	Tables S6 and S8	0.05	ton	Tables S6 and S13	0.05	ton	Tables S6 and S19
Sodium chloride	0.66	ton	Tables S6 and S8	0.66	ton	Tables S6 and S13	0.66	ton	Tables S6 and S19
Ultrapure water	2.20	ton	Tables S6 and S8	2.20	ton	Tables S6 and S13	2.20	ton	Tables S6 and S19
N_2	0.08	ton	Tables S6 and S8	0.08	ton	Tables S6 and S13	0.08	ton	Tables S6 and S19
H_2	0.01	ton	Tables S6 and S8	0.01	ton	Tables S6 and S13	0.01	ton	Tables S6 and S19
Decarbonized air	1.21	ton	Tables S6 and S8	1.21	ton	Tables S6 and S13	1.21	ton	Tables S6 and S19
Disposal									
Aluminum	–			128	ton	The aboveground treatment facilities were scaled up to 160 times of the example system in (Ding et al., 2022).	–		
Steel	–			480	ton		–		
HDPE	–			264	ton		–		
GAC	–			144	ton		–		
PVC pipe	–			64	ton		–		
Concrete	–			9680	ton		–		
Energy consumption									
Construction	3850904	kWh	Tables S9 and S11	3400	kWh	Tables S14 and S16	2096.75	kWh	Tables S20 and S22
Operation	–			2207520	kWh	Tables S14 and S16	–		
Sampling and analysis	66.05	kWh	Tables S9 and S11	66.05	kWh	Tables S14 and S16	66.05	kWh	Tables S20 and S22
Disposal	–			8332800	kWh	Tables S14 and S16	–		
Transportation									
Materials	4627199.29	tkm	Table S10	657115.14	tkm	Table S15	149192.01	tkm	Table S21
Equipment	500660	tkm	Table S10	5030	tkm	Table S15	4218.61	tkm	Table S21
People	1360	pkm	Table S10	4000	pkm	Table S15	4000	pkm	Table S21

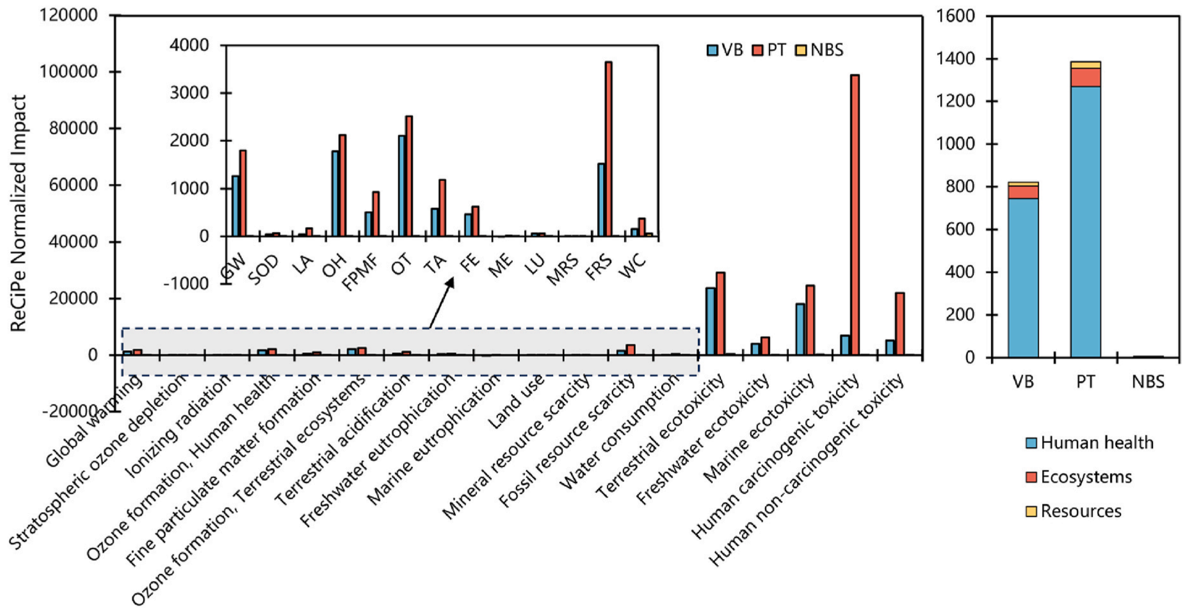


Fig. 4. Normalized impacts results for each scenario. (detail information see in Supporting Information S4). GW: global warming; SOD: stratospheric ozone depletion; LA: ionizing radiation; OH: ozone formation, human health; FPMF: fine particulate matter formation; OT: ozone formation, terrestrial ecosystems; TA: terrestrial acidification; FE: freshwater eutrophication; ME: marine eutrophication; LU: land use; MRS: mineral resource scarcity; FRS: fossil resource scarcity; WC: water consumption.

aboveground wastewater treatment systems, which is a major contributor to the carbon footprint of PT, thus resulting in comparable total carbon emissions between two studies despite the variations in design of the extraction system. The superior performance of BPABs (332.91 kg CO_2-eq/kg) compared with VB systems in this study (4391.81 kg CO_2-eq/kg) further validates the greater decarbonization potential of green material substitution than traditional cement-based ones.

Notably, existing LCAs of phytoremediation remain sparse, particularly for benzene-contaminated aquifers. O'Connor et al. achieved a total net environmental benefit of 834 Pt through the planting of 425 eucalyptus over an area of 9000 m^2 (comparable density to this study) in their phytoremediation for a tetrachloroethylene-contaminated aquifer (O'Connor and Hou, 2020), which falls significantly below the anticipated impact of NBS in our study. This disparity arises from the fact that in their scenario, the biomass was utilized as saw timber, effectively serving as carbon storage, thus rendering a net environmental benefit. This also explains why, in this study, phytoremediation exhibited a larger impact than the traditional alternative in certain impact categories, such as marine eutrophication, as the full potential of biomass utilization for environmental gains may not have been fully realized.

The LCIA also revealed variations in environmental performance rankings across different impact categories among the evaluated alternatives. These discrepancies partly arise from uncertainties introduced by simplified inventory data, as well as methodological sensitivities of the ReCiPe Midpoint assessment. As shown in Fig. 4, Table S27 and Table S28, VB is seen to have the largest negative impact on land use category among the compared alternatives in the ReCiPe Midpoint assessment; but it also has the lowest impact in categories such as marine eutrophication; the PT option has the largest impact score in most other impact categories. Overall, despite the uncertainties of each alternative, NBS is clearly ranked as the remediation that best maximizes net environmental benefits. While all 18 midpoint categories under ReCiPe were included to capture broader impacts, results for regionalized categories such as land and water use carry greater uncertainty owing to methodological simplifications and regionalized assumptions. The main conclusions of this study are primarily grounded in more robust categories, particularly climate change and energy use.

3.2. *Contribution analysis and improvement options*

Process contribution analysis identified the dominant components in each remediation scenario. The percent contribution and the tree diagrams are shown in Fig. 5 and Fig. S9–S11, respectively.

VB impacts are predominantly attributed to material consumption, particularly cement, which accounts for approximately 95 % of impacts in certain categories. This high contribution is largely due to the substantial cement demand, as cement production is both energy-intensive and emission-intensive, involving both high-temperature fuel combustion and calcination of limestone and releasing significant quantities of CO_2. The high resource intensity of cement also contributes significantly to the resource depletion category (Fig. 5), while associated emissions from production and transport affect both human health (e.g., fine particulate matter) and ecosystem quality (e.g., acidification and eutrophication). To mitigate the environmental burden of VB-based remediation, optimizing the type, performance, and production processes of barrier filler materials is imperative. Previous studies, such as those by Tabbaa et al., have also highlighted cement as the most significant cost component in VB construction et al., 2021; Cao et al. (2024); Cao et al. (2022). Transportation emerges as another essential contributor, particularly in ecotoxicity-related categories, due to the off-hauling of waste to landfills. These results align with those of previous LCA studies, which emphasize the significant role of transportation in off-site disposal impacts (Li et al., 2020; Ram et al., 2020; Sandanayake et al., 2019). Addressing this impact could involve the adoption of fuel-efficient, low-emission vehicles and alternative fuels with reduced life cycle emissions. Overall, the results reveal that the upstream phases of the VB scenario, encompassing material acquisition and transportation, contribute substantially across all impact categories. In contrast, downstream, including barrier operation and monitoring, demonstrate negligible environmental impacts. These findings align with typical characteristics of passive remediation systems, where material requirements during preparatory phases generally outweigh the operational energy consumption (Hou, 2020; Vocciante et al., 2021).

Similarly, in the PT scenario, the use of energy-intensive materials such as steel in pumping infrastructure and concrete for construction also contributes notably to the total emissions, as these materials are

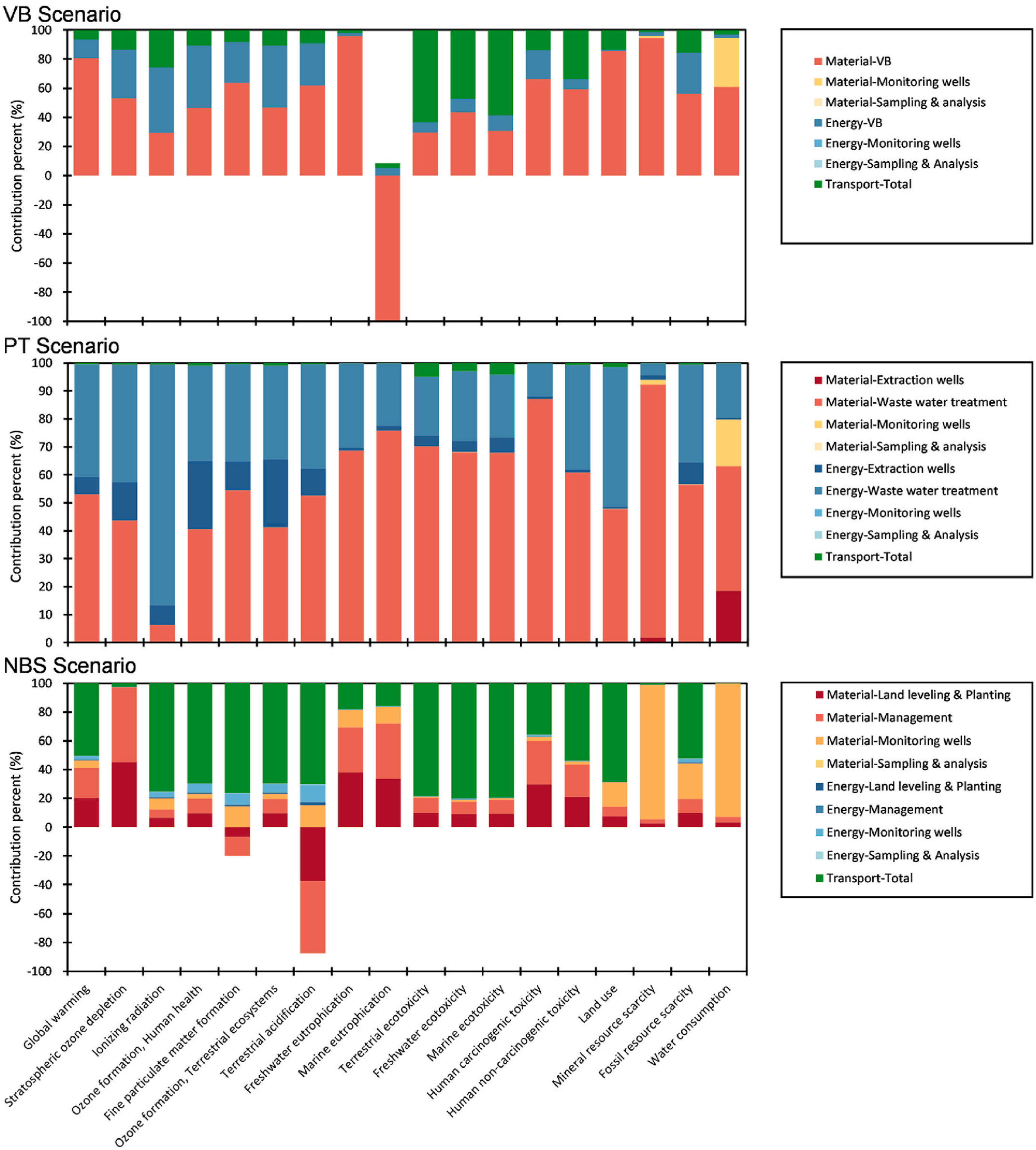


Fig. 5. The percent contribution of transportation, material and energy consumption of three assessed scenarios to each impact category.

associated with fossil fuel-based manufacturing processes and high embodied energy. What is different from the VB scenario is that the material and energy consumption in PT scenario exhibits a comparable level of contribution. Notably, wastewater treatment, as a distinct subsystem, basically dominates both material and energy consumption, accounting for over 50 % of the impact across all categories. This reflects the substantial resource and energy demands of treating large volumes of extracted groundwater, particularly for chemical and physical treatment processes. These processes often involve continuous operation of energy-intensive equipment such as pumps, blowers, and reactors, which substantially contribute to carbon emissions when powered by conventional energy sources. Therefore, optimizing the performance parameters and minimizing the quantities of agents used in wastewater treatments, such as coagulants, adsorbents, and oxidants, represents a critical opportunity for reducing the carbon footprint of this technology. In addition, improving energy efficiency can directly reduce the life

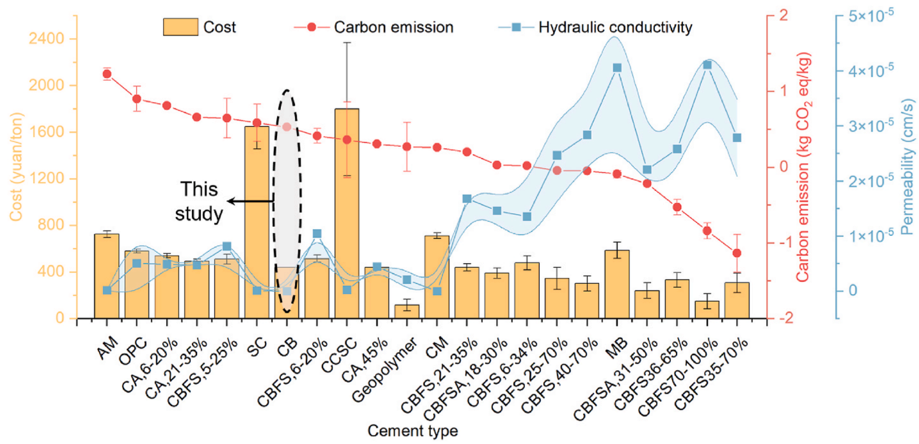


Fig. 6. Sensitivity analysis of functional materials for subsystems. AM: Adhesive mortar; OPC: Ordinary Portland cement; CA, 6–20 %: Cement, alternative constituents 6–20 %; CA, 21–35 %: Cement, alternative constituents 21–35 %; CBFS, 5–25 %: Cement, blast furnace slag 5–25 %; SC: Sulfolauminate cement; CB: Cement-Bentonite; CBFS, 6–20 %: Cement, blast furnace slag 6–20 %; CCSC: Carbonatable Calcium Silicate cement (Solidia); CA, 45 %: Cement, alternative constituents 45 %; CM: Cement mortar; CBFS, 21–35 %: Cement, blast furnace slag 21–35 %; CBFSA, 18–30 %: Cement, blast furnace slag 18–30 % and 18–30 % other alternative constituents; CBFS,6–34 %: Cement, blast furnace slag 6–34 %; CBFS,25–70 %: Cement, blast furnace slag 25–70 %; CBFS,40–70 %: Cement, blast furnace 40–70 %; MB: Magnesia Binder; CBFSA,31–50 %: Cement, blast furnace slag 31–50 % and 31–50 % other alternative constituents; CBFS36-65 %: Cement, blast furnace slag 36–65 %; CBFS70-100 %: Cement, blast furnace slag 70–100 %; CBFS35-70 %: Cement, blast furnace slag 35–70 %.

cycle environmental footprint by lowering the electricity demand per unit of treated water, which decreases upstream emissions associated with fossil fuel-based power generation. Enhanced process control and efficient equipment also reduce heat loss and auxiliary energy use (e.g., for chemical preparation or thermal regulation), thereby minimizing indirect emissions. These efficiency gains help limit both greenhouse gas emissions and other impact categories such as fine particulate matter formation and photochemical ozone creation. Hence, adopting energy-efficient treatment technologies (e.g., membrane bioreactors with low-energy configurations), improving system control to avoid over-treatment, and integrating on-site renewable energy (e.g., solar-assisted aeration) can improve the environmental performance of PT systems by lowering operational energy demand and associated emissions, thereby further enhancing the sustainability of PT systems.

In contrast, in the NBS scenario, the use of naturally derived materials, such as poplar trees, generates minimal impacts during installation stage due to the low resource intensity of planting activities. However, the operational stage of the NBS, including transportation and monitoring that required to ensure system stability and performance, drives impacts in categories such as ecotoxicity and human health. To be specific, transportation contributes up to 80 % of impacts in most categories, reflecting the substantial emissions associated with transporting plant substrates and related materials to the site. And monitoring activities contribute up to 95 % of the total impact, particularly in resource-related categories such as mineral resource scarcity and water consumption. This is consistent with findings from other studies on nature-based systems, where maintenance and operational activities constitute a significant share of the overall environmental burden (Alshahrani et al., 2022; Nika et al., 2020). Optimization may include local sourcing of fertilizer and other required materials, consolidation of shipments, and adoption of low-emission transportation modes such as electric or biodiesel-fueled vehicles. Additionally, fertilizer use in daily management also slightly contributes to ecosystem-related categories such as eutrophication and acidification, but its share is notably lower than in agricultural systems (Brousseau et al., 2024; Jiang et al., 2021; Krzyżaniak et al., 2019; Pradel et al., 2020). This is due to the low nutrient demands of poplar species, which have long growth cycles and inherent resilience, reducing fertilizer input requirements. Compared to systems with intensive fertilizer use, such as high-input agricultural practices, the reduced reliance on fertilizers in this study significantly lowers the associated environmental burden. Notably, the NBS scenario demonstrates unique net environmental benefits in categories such as fine particulate matter formation and terrestrial acidification, as shown in Fig. 5. These benefits are likely driven by the carbon sequestration capabilities of plants and soil amendments, which capture airborne pollutants and neutralize acidifying compounds in the surrounding environment. Optimizing biomass utilization could further enhance these benefits. For example, converting harvested plant residues into bioenergy or leveraging them for long-term carbon storage could offset emissions from transportation and monitoring activities (Adler et al., 2022; Carvalho et al., 2022; Heidari et al., 2019; O'Connor and Hou, 2020). These findings highlight the dual role of NBS as both a remediation strategy and a mechanism for environmental improvement, emphasizing its potential to align remediation efforts with broader ecological restoration and carbon reduction goals. This distinct advantage underscores the value of integrating NBS into sustainable remediation frameworks, particularly in settings where co-benefits such as ecosystem enhancement and emissions reduction are priorities.

3.3. *Optimization strategies for enhanced sustainability*

3.3.1. *Multi-objective optimization of VB scenario: balancing containment control, carbon footprint, and cost efficiency*

The LCA identifies cement production as the primary contributor to GHG emissions in VB systems, accounting for 80–90 % of total emissions across the construction phase. Hence, optimizing the barrier filling materials for the barrier can significantly reduce both environmental and economic impacts.

One viable solution is the adoption of "green" cement. The substitution of ordinary Portland cement (OPC) with industrial byproducts like ground granulated blast-furnace slag (GGBS) presents a promising pathway for emission reduction, with potential GHG savings of 0.58–0.82 t CO_2-eq per ton of cement replaced (Li et al., 2020; Reddy et al., 2024). However, our permeability analysis reveals that GGBS-based mixtures exhibit hydraulic conductivity values (1.5-3.0 $\times 10^{-7}$ m/s) nearly an order of magnitude higher than conventional OPC systems (1.0×10^{-8} m/s) (Elkhaldi et al., 2022; Paruthi et al., 2024; Singh et al., 2023). This technical compromise creates a paradoxical scenario where achieving equivalent containment performance requires 20–35 % greater material volumes, thereby offsetting 40–60 % of the initial carbon savings. Another approach is to reduce the material dosage. Recent advances in reactive barrier materials suggest potential

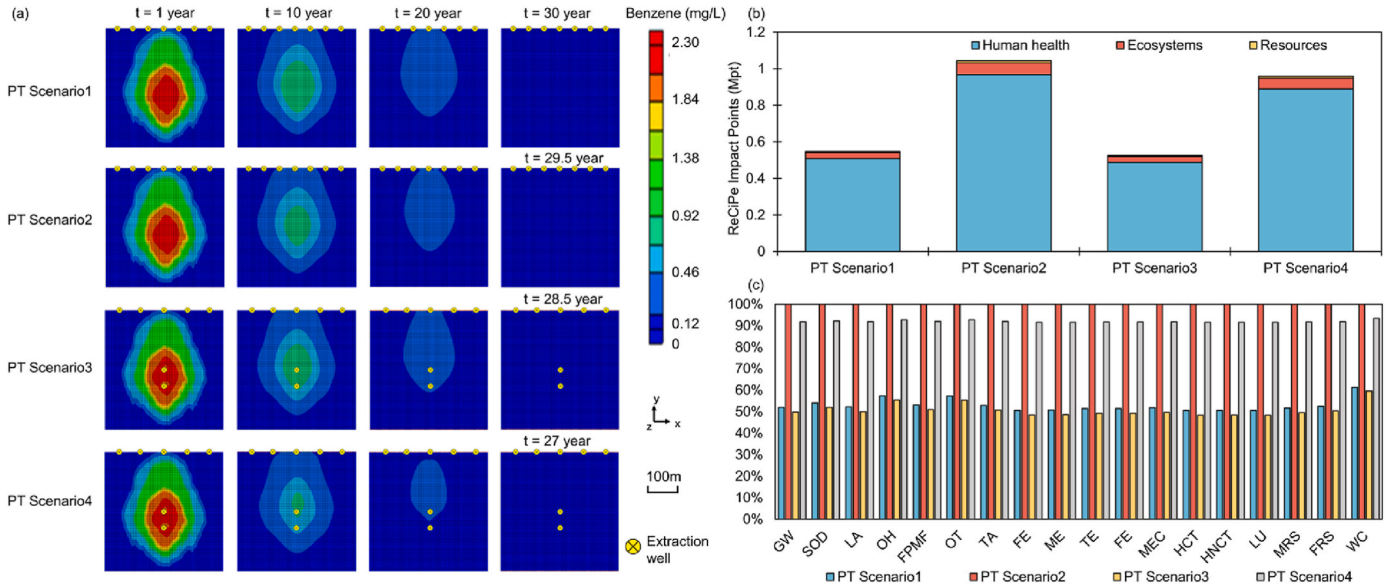


Fig. 7. Life cycle environmental impacts of 4 PT scenarios with varying well arrangements and extraction intensities. (a) GMS modeling results; (b) endpoint assessment; (c) midpoint assessment.

solutions to this optimization challenge. Biochar-amended bentonite composites, for instance, demonstrate synergistic improvements in both permeability and benzene adsorption efficiency (~40 %) compared to traditional OPC mixtures (Alshahrani et al., 2022; Budania and Dangayach, 2023; Lyu et al., 2020). Such innovations enable 30–50 % reductions in wall thickness while maintaining equivalent containment efficacy, though at 2–3 higher material costs.

Our supplementary meta-analysis (Fig. 6, Table S24) of 17 barrier projects over the past five years, both domestically and internationally, identifies a critical trade-off frontier between material sustainability indices and technical performance metrics. We encompassed three critical parameters: hydraulic containment performance, carbon intensity reduction, and economic feasibility. As illustrated in Fig. 6, while modified materials enhance hydraulic containment performance to some extent, they may compromise environmental friendliness. Conversely, green materials often underperform OPC in terms of permeability. Therefore, identifying an optimal balance between three critical parameters of barrier filling materials is crucial for minimizing both environmental and economic burdens of remediation efforts.

These findings underscore the necessity for context-specific optimization frameworks in VB design. A proposed three-tier decision hierarchy could prioritize: (1) site-specific hydrogeological conditions dictating minimum permeability requirements, (2) locally available alternative cementitious materials determining carbon reduction potential, and (3) life-cycle cost constraints governing final material selection. Multi-criteria decision analysis shows particular promise in navigating this complex optimization space, particularly for groundwater benzene plumes requiring long-term containment.

3.3.2. Adaptive wellfield design for PT scenario: aligning hydraulic control with environmental performance

The original PT scenario applied a conventional edge-barrier configuration, with seven extraction wells uniformly arranged along the downgradient plume boundary, each operating at 5 m^3/day. Solute transport modeling showed this configuration required 30 years to achieve target benzene reductions.

Increasing individual well flow to 10 m^3/day slightly reduced remediation time to 29.5 years, but with limited efficiency gain relative to the increased energy input. This prompted a spatial optimization strategy: five wells were retained along the plume edge, and two relocated to the source zone to enhance mass removal at the origin. This

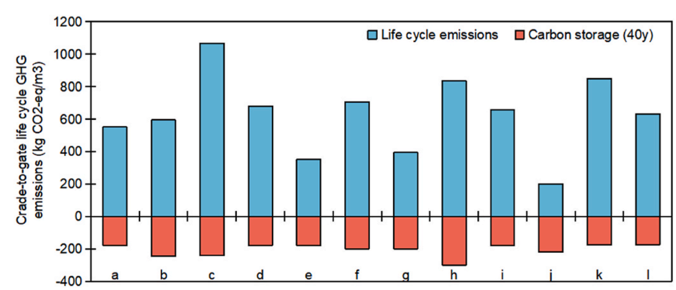


Fig. 8. Comparison of cradle-to-gate life cycle GHG emissions and carbon storage (a. this study; b. (O'Connor and Hou, 2020); c.(Adler et al., 2022); d. (Hafezi et al., 2021); e. (Kouchaki-Penchah et al., 2016); f. (Puettmann et al., 2016); g. (Piekarski et al., 2017); h (Nakano et al., 2018). and i.(Puettmann et al., 2013). Note that differences between studies shown here can partly be attributed to the fact that standards for fiberboards differ from country to country.

dual-zone layout shortened remediation to 28.5 years at 5 m^3/day, and to 27 years at 10 m^3/day.

LCA of the four configurations (Fig. 7) showed that the optimized layout with moderate flow (PT Scenario3) achieved the lowest environmental impacts. This is largely attributable to reduced cumulative pumping and chemical treatment demands, consistent with the contribution analysis identifying reagent usage as a key impact driver for PT systems.

Our LCA-integrated modeling approach extends this paradigm by demonstrating that strategic spatial reconfiguration can deliver both performance and sustainability benefits, offering a practical pathway to improving the real-world application of PT systems.

3.3.3. Biomass utilization and carbon storage in NBS scenario: from carbon neutrality to net-negative systems

Conventional LCA frequently underestimates NBS carbon benefits by oversimplifying or even neglecting biomass utilization (Hafezi et al., 2021). Previous studies (O'Connor and Hou, 2020; Vigil et al., 2015) have demonstrated that phytoremediation systems may underperform traditional remediation methods when biomass is discarded post-harvest, but they exhibit superior environmental performance when biomass is strategically repurposed. Instead of discarding the

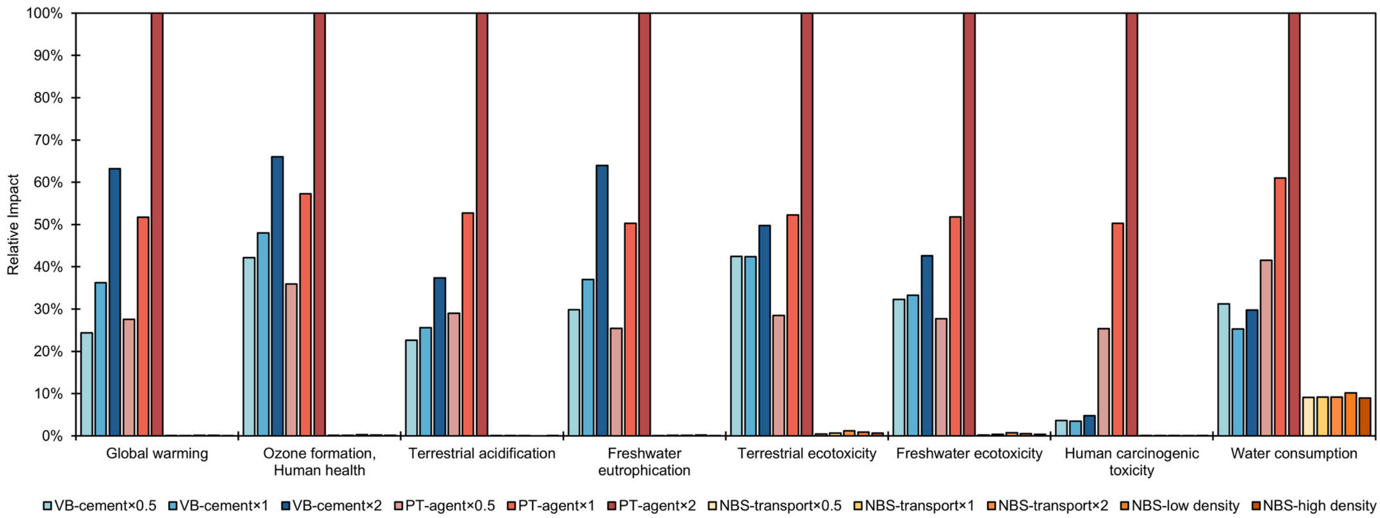


Fig. 9. Sensitivity analysis of the key parameters.

harvested poplar trees post-remediation, which would diminish their environmental value, we consider their conversion into medium-density fiberboard (MDF), a durable wood product with long-term carbon retention capacity. Following established studies (Hafezi et al., 2021), we model the cradle-to-grave greenhouse gas footprint of poplar-based MDF, including emissions from harvesting, processing, transportation, and end-use, as well as the biogenic carbon retained over a 40-year product lifespan. Detailed calculations are listed in Section 4.3 in SI.

Our results indicate a net carbon storage of -180 kg CO_2-eq/m^3 of fiber, reflecting the combined benefits of material substitution and long-term sequestration in MDF. These findings underscore the importance of integrating biomass end-use pathways in the life cycle modeling of nature-based remediation systems. By accounting for carbon flows beyond the remediation phase, the NBS scenario demonstrates the potential to transition from carbon neutrality toward carbon-negative performance, supporting broader sustainability goals.

Moreover, comparative analysis of cradle-to-gate GHG emissions (Fig. 8, Table S26) indicates that poplar-based MDF exhibits emissions comparable to or lower than those of conventional fiberboard alternatives. Notably, despite its shorter growth cycle (12–15 years), poplar achieves higher cumulative carbon storage than long-rotation species (10–90 years), owing to more frequent harvesting and regeneration cycles. Crucially, our analysis advances existing frameworks by incorporating rotation and storage periods, a methodological gap in earlier research, thereby providing a more holistic evaluation of poplar's carbon mitigation potential.

3.4. Sensitivity analysis for environmental impacts

A sensitivity analysis was conducted to assess how variations in input parameters influence the consequent environmental impacts (Fig. 9). The analysis focused on critical parameters across three distinct scenarios: materials for barrier construction, reagent dosage for wastewater disposal and transport distance.

Cement usage in the VB system shows significant influence across multiple impact categories. When the cement quantity is doubled, the environmental impacts in categories such as global warming, ozone formation, and freshwater eutrophication increase dramatically, even exceeding those of the PT scenario. This underscores the considerable carbon footprint associated with high cement usage in VB, presenting an unexpected disadvantage relative to the PT scenario in these specific impact categories. Conversely, halving the cement content reduces the impact scores in all categories, though VB still generally exhibits higher impacts than the NBS scenario.

In the PT scenario, a 50 % reduction in chemical agent use lowers impact scores in certain categories, notably making PT impacts even lower than VB in global warming, ozone formation, freshwater eutrophication, and terrestrial/freshwater ecotoxicity. Despite this reduction, however, the overall ranking in most impact categories remains unchanged, with PT still exhibiting higher impacts than NBS and comparable or slightly higher impacts than VB in many cases.

The NBS scenario demonstrates strong environmental robustness across varied implementation parameters. Beyond transportation, we tested design variations that reflect different land-use constraints and planting configurations, as a means of assessing spatial adaptability. Despite these changes, NBS maintained the lowest impact scores across all categories, highlighting its potential and suitability as an environmentally sustainable remediation approach. Nevertheless, in transitioning from modeled scenarios to applications, practical constraints such as soil suitability, potential disturbance from active infrastructure or underground pipe network, and compatibility with site redevelopment plans may restrict the feasibility of NBS at operating industrial sites, underscoring the importance of site-specific assessment of this strategy.

4. Conclusion

This study for the first time applied LCA to evaluate groundwater remediation at active industrial areas, focusing on three distinct strategies: VB, PT and an innovative NBS incorporating phytoremediation. Our findings highlight that NBS, particularly with biomass utilization, delivers remarkable net environmental benefit, significantly reducing GHG emissions compared to conventional remediations. The LCA results reveal critical processes contributing to the overall environmental footprint of each remediation strategy. For VB and PT, energy-intensive processes such as construction and operation of barriers and pumps dominate the emissions. In contrast, the NBS scenario benefits significantly from carbon storage through biomass valorization, which offsets the emissions basically driven by monitoring activities. The study also explores sustainable material alternatives such as "green" cement in VB systems, revealing trade-offs between containment performance, carbon reduction, and cost efficiency; in the PT scenario, spatial and operational optimization of well placement and flow rates further demonstrates opportunities to reduce environmental burdens while maintaining remediation effectiveness.

In conclusion, this study provides a robust methodological basis and practical insights for the adoption of low-carbon and NBS in groundwater remediation. The proposed framework holds great potential for advancing sustainable remediation practices and fostering the transition toward a greener and more resilient future. While this study is grounded in a benzene-contaminated industrial site, the proposed framework is adaptable to other pollutants and site conditions. Future work will aim to enhance regional specificity and incorporate broader sustainability dimensions, such as economic feasibility and social acceptance, toward more holistic assessments of low-carbon, nature-based remediation strategies.

CRediT authorship contribution statement

Han Xu: Writing – original draft, Methodology, Investigation. **Deyi Hou:** Writing – review & editing, Supervision, Project administration, Methodology, Funding acquisition.

Declaration of competing interest

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

Acknowledgments

This work was supported by the National Key Research and Development Program of China (Grant No. 2022YFC3703302) and the National Natural Science Foundation of China (Grant No. 42225703).

Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.jclepro.2025.146697.

Data availability

Data will be made available on request.

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