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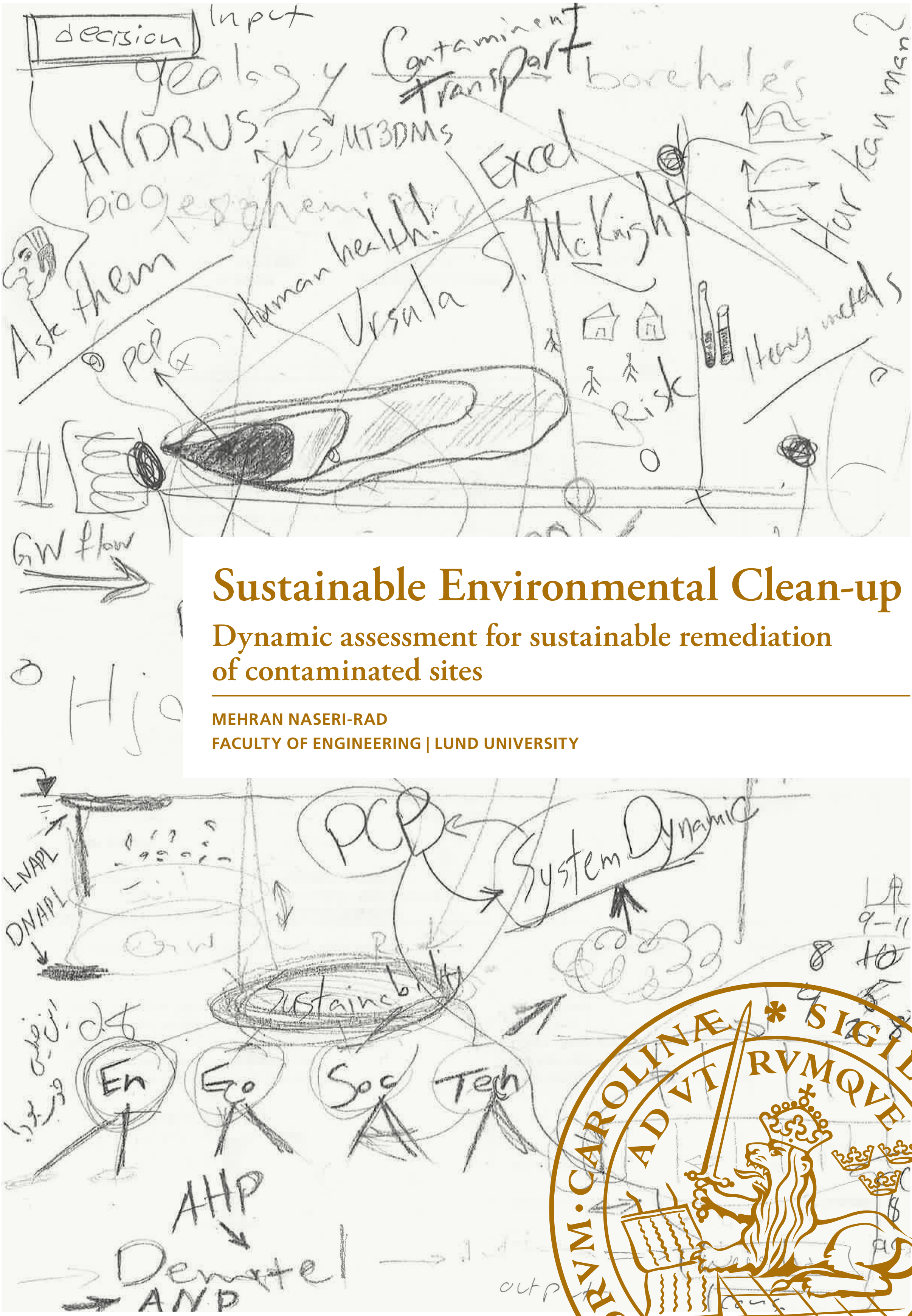

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Dynamic assessment for sustainable remediation of contaminated sites

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FACULTY OF ENGINEERING | LUND UNIVERSITY

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Mehran Naseri-Rad

DOCTORAL DISSERTATION

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Abstract

Soil and groundwater contamination is an increasingly recognised threat to public health and the environment around the globe. New types of contaminants continue to emerge, and awareness of their threat, continues to develop. Many countries have national clean-up programs with priority lists of the most hazardous contaminated sites. Investigation and remediation of these sites, however, take a long time. An important reason is that dealing with contaminated sites has high practical complexity and uncertainty, making it hard to decide whether a specific remedy measure should be implemented. This depends not only on hydrological and biogeochemical heterogeneities and variabilities at a site, but also on associated health, environmental, economic, and social impacts of taking or not taking an action in the long run. Contaminant fate and transport models help to understand and predict subsurface behaviour and potential risks. As well, sustainability assessment tools can help in the decision-making process. These tools aim at quantifying environmental, economic, and social impacts and comparing different scenarios of remediation to give an overview of all potential impacts with time. However, integration of contaminant transport models and sustainability assessment tools has not been performed, leading to a lack of a holistic but pragmatic view of the whole system. This could admittedly result in fixing one problem while generating new ones. Thus, this thesis integrates these into a novel system that recognizes variations of involved factors in time. For this, a contaminant transport model (INSIDE-T) and a sustainability assessment tool (INSIDE) were developed with the aim of coupling through a system dynamics approach and simulations, for its unique capabilities in integrating multiple types of data/information sources. This integration can provide a holistic, but pragmatic guide for decision-making in remediation actions. The new tool, DynSus, enables site managers to assess consequences of their decisions in site clean-up projects in terms of contaminant spread risk, social, environmental, and economic impacts from a dynamic life cycle perspective. For this, experience from experienced site managers and stakeholders is used and the methodology is implemented, among others, on a seriously contaminated site in Sweden overseen by the Swedish Geological Survey as the main case study of the thesis. The results show that ”gentle” remedy measures, which are often considered sustainable, may not be the best options in terms of life cycle impacts, although they generally gain significantly higher sustainability scores at the beginning of the remediation process. The time these measures rank below more invasive methods is calculated by DynSus.

Key words: contaminated sites, sustainability assessment, remediation, multicriteria decision analysis, system dynamics, contaminant transport

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"This world is a mountain,
and our actions a shout;
Like it or not,
the echo of the shout is to come back to us."

-Rumi (Persian poet, 1207-1273 A.D.)

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Acknowledgement

This thesis is all about interactions of involved factors in a system and their influence and importance in forming a system's behaviour. Taking the journey of this thesis as a system, there are certainly so many amazing people who were truly influential and important factors throughout the process, without whom there would not be the current system (thesis) at all! So, I would like to take this opportunity to thank them all.

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Abstract

Soil and groundwater contamination is an increasingly recognised threat to public health and the environment around the globe. New types of contaminants continue to emerge, and awareness of their threat, continues to develop. Many countries have national clean-up programs with priority lists of the most hazardous contaminated sites. Investigation and remediation of these sites, however, take a long time. An important reason is that dealing with contaminated sites has high practical complexity and uncertainty, making it hard to decide whether a specific remedy measure should be implemented. This depends not only on hydrological and biogeochemical heterogeneities and variabilities at a site, but also on associated health, environmental, economic, and social impacts of taking or not taking an action in the long run. Contaminant fate and transport models help to understand and predict subsurface behaviour and potential risks. As well, sustainability assessment tools can help in the decision-making process. These tools aim at quantifying environmental, economic, and social impacts and comparing different scenarios of remediation to give an overview of all potential impacts with time. However, integration of contaminant transport models and sustainability assessment tools has not been performed, leading to a lack of a holistic but pragmatic view of the whole system. This could admittedly result in fixing one problem while generating new ones. Thus, this thesis integrates these into a novel system that recognizes variations of involved factors in time. For this, a contaminant transport model (INSIDE-T) and a sustainability assessment tool (INSIDE) were developed with the aim of coupling through a system dynamics approach and simulations, for its unique capabilities in integrating multiple types of data/information sources. This integration can provide a holistic, but pragmatic guide for decision-making in remediation actions. The new tool, DynSus, enables site managers to assess consequences of their decisions in site clean-up projects in terms of contaminant spread risk, social, environmental, and economic impacts from a dynamic life cycle perspective. For this, experience from experienced site managers and stakeholders is used and the methodology is implemented, among others, on a seriously contaminated site in Sweden overseen by the Swedish Geological Survey as the main case study of the thesis. The results show that ”gentle” remedy measures, which are often considered sustainable, may not be the best options in terms of life cycle impacts, although they generally gain significantly higher sustainability scores at the beginning of the remediation process. The time these measures rank below more invasive methods is calculated by DynSus.

Popular science summary

Industrial revolution and continuous increasing demand for chemical products supply for different types of goods have left a legacy of millions of contaminated soil and groundwater sites around the globe. It is estimated that there are about three million potentially contaminated soil and groundwater sites in Europe. Managing this big number of sites costs billions of euros every year and clean-up of these is expected to take several decades at the current pace. Different countries have different strategies and plans for accelerating the clean-up process. In Sweden, there are some 80,000 potentially contaminated sites, of which about 8,000 are classified in risk class 1 or 2 by the Swedish Environmental Protection Agency. This means that they can induce "very high" or "high" risk to human health or the environment, respectively. According to "A non-toxic environment", which is one of the sixteen environmental quality goals of the Swedish environmental policy, all these sites must be remediated by 2050. At the current pace, however, this is estimated to take a much longer time (some 150 years). One reason for this low pace is the high complexity and inherent uncertainty in subsurface media that is caused by high hydrologic and biogeochemical heterogeneity and variability. From a technical point of view, this makes it hard to decide which remedy action to take and how, because it is difficult to reliably estimate how far and how long the contamination plume will spread.

Cost, time, and complex hydrogeochemical dynamics are, however, not the only problems in this regard. The potential risk for public health in case of late or insufficient action causes social pressure on decision-makers. Even taking remedial action is not necessarily beneficial. It could inversely impact the local environment so that the overall environmental benefit would be less than the unwanted impacts (e.g., carbon emission, waste generation). Added to these direct issues, there are indirect considerations like reduced land price surrounding contaminated areas and reduced mental well-being of residents. Consequently, this is a multidimensional and multidisciplinary problem with many stakeholders.

To help with this complex problem, several decision support tools have been introduced. These tools are either focusing on technical aspects of the problem in terms of contaminant transport modelling or focusing on managerial aspects in terms of sustainability assessment tools (i.e., in different types of economic, social, or environmental impact assessment and more commonly, a combination of these three). Contaminant fate and transport models simply try to assess the associated risk of the contamination in question by calculating how far the contaminant plume can spread, basically regardless of other aspects of the problem. Sustainability assessment tools, on the other hand, try to describe how sustainable taking action will affect sustainability (in terms of economic, social, and environmental impacts), regardless of contamination plume change patterns in time and space. Contaminant transport models and sustainability assessment tools are seldom integrated properly to fill this gap, simply because they are focussing on different tasks, disregarding what decision-makers really need. Such a problem is beyond single disciplines and difficult for decision-makers to handle without reliable and transparent support. Thus, there is a need for more holistic approaches that can consider all aspects of the problem.

In view of the above, the aim of this thesis is to fill this gap by initiating novel versatile support tools that consider all aspects of the problem and their dynamics by integrating contaminant transport modelling with sustainability assessment tools. For this purpose, a new type of transport model and sustainability assessment tool is introduced and evaluated. System dynamics simulations are used for the integration of its capabilities in taking different types of data and interrelations among sub-systems to give rise to a more holistic approach. This provides a more realistic and dynamic picture of the whole remediation system that recognizes the field dynamics in a life cycle perspective. The new tool was developed by communicating with site managers and performing trials and tests to verify the applicability of the tool. A contaminated site was chosen as the main site in this thesis for developing the contaminant transport model and the final overall tool. The site is a former sawmill plant in Hjortsberga, Alvesta Municipality, Kronoberg County, southern Sweden. The sawmill plant was in operation from the early 1940s to the late 1970s and has left a legacy of contaminated soil and groundwater with pentachlorophenol (PCP). Contaminated soil at the site has already been removed, but the contamination in groundwater is threatening the nearby Lake Sjöatorpasjön. Also, for developing the basic sustainability assessment tool, a heavy metal contaminated groundwater site in southwestern Iran and a petrochemical contaminated site in Kazakhstan was chosen for testing the transport model in a bigger scale. The dynamic assessment of these experimental sites shows that the assumed life cycle sustainability of a remediation technology may not be really optimal over time. Also, certain remediation technologies may show very low sustainability at the beginning of the remediation project but compensate the overall negative impacts faster than expected and provide higher life cycle sustainability.

Summary in Persian – چکیده ی رساله

انقلاب صنعتی و تقاضای فزاینده مستمر برای عرضه محصولات شیمیایی برای انواع مختلف فعالیت ها میراثی از میلیون ها سایت آلوده (مناطقی با خاک و آب زیرزمینی آلوده) در سراسر جهان به جا گذاشته است. تخمین زده می شود که حدود سه میلیون سایت آلوده بالقوه در اروپا وجود دارد. مدیریت این تعداد زیاد سایت ها سالانه میلیاردها یورو هزینه دارد و انتظار می رود پاکسازی آنها با سرعت فعلی چندین دهه به طول بیانجامد. کشورهای مختلف استراتژی ها و برنامه های متفاوتی برای تسریع روند پاکسازی دارند. در سوئد، حدود 80،000 سایت بالقوه آلوده وجود دارد که آژانس حفاظت از محیط زیست سوئد حدود 8،000 سایت از این تعداد را در کلاس خطر 1 یا 2 طبقه بندی کرده است. این بدان معنی است که آنها می توانند به ترتیب خطر "بسیار زیاد" یا "زیاد" ی را برای سلامت انسان یا محیط زیست ایجاد کنند. با توجه به "محیط زیست غیر سمی" که یکی از شانزده هدف کیفیت زیست محیطی در سیاست زیست محیطی بالادستی در سوئد است، همه این سایت ها باید تا سال 2050 پاکسازی شوند. با این حال، با سرعت کنونی، تخمین زده می شود که نیل به چنین هدف بلندی زمان بسیار بیشتری طول بکشد (حدود 150 سال). یکی از دلایل این سرعت پایین، پیچیدگی بالا و عدم قطعیت ذاتی در محیط های زیر سطحی است که ناشی از ناهمگونی و تنوع هیدرولوژیکی و بیوژئوشیمیایی بالا در محیط اشباع و غیر اشباع است. از نقطه نظر فنی، این امر تصمیم گیری در مورد اینکه چه روش پاکسازی و به چه صورت انجام شود را دشوار می کند، زیرا تخمین این که توده آلودگی تا کجا و به چه مدت به پیشرفت و گسترش خود ادامه می دهد، کاری دشوار است.

هزینه، زمان و پویایی عوامل هیدروژئوشیمیایی، تنها مشکلات موجود در این زمینه نیستند. خطر بالقوه برای سلامت عمومی در صورت اقدام دیرهنگام یا ناکافی باعث فشار اجتماعی بر تصمیم گیرندگان می شود. حتی انجام اقدامات اصلاحی لزوماً سودمند نیست. چنین پروژه هایی می توانند بر محیط محلی تأثیر معکوس بگذارد به طوری که در مجموع منافع زیست محیطی کمتر از تأثیرات ناخواسته بر محیط زیست (به عنوان مثال انتشار کربن، تولید زباله) باشد. علاوه بر این، ملاحظات غیرمستقیم مانند کاهش قیمت زمین در اطراف مناطق آلوده و کاهش رفاه روانی ساکنان محلی وجود دارد. در نتیجه، این یک مشکل چند بعدی و دامنه دار با طیف وسیعی از ذینفعان است.

برای کمک به حل این مشکل، چندین ابزار پشتیبانی تصمیم گیری معرفی شده است. این ابزارها یا بر جنبه‌های فنی مشکل از نظر مدل سازی انتقال و انتشار آلاینده یا بر جنبه‌های مدیریتی از نظر ابزارهای ارزیابی پایداری (sustainability assessment) تمرکز می‌کنند (به عنوان مثال، انواع مختلف ارزیابی اثرات اقتصادی، اجتماعی یا زیست‌محیطی و معمولاً ترکیبی از این سه). مدل‌های انتقال و انتشار آلاینده صرفاً سعی می‌کنند خطرات مرتبط با آلودگی مورد نظر را با محاسبه میزان انتشار توده آلاینده، اساساً بدون توجه به سایر جنبه‌های مشکل، ارزیابی کنند. از سوی دیگر، ابزارهای ارزیابی پایداری تلاش می‌کنند تا توصیف کنند که هرگونه اقدام برای پاکسازی آلودگی چه تأثیری بر پایداری (از نظر تأثیرات اقتصادی، اجتماعی و زیست‌محیطی) می‌گذارد. تاکنون مدل‌های انتقال و انتشار آلاینده و ابزارهای ارزیابی پایداری برای ایجاد این حلقه مفقوده به درستی ادغام نشده اند، صرفاً به این دلیل که بر کارکردهای تعریف شده برای خود تمرکز می‌کنند، بدون توجه به آنچه تصمیم گیرندگان برای مسائل واقعی

نیاز دارند. چنین مشکلی فراتر از زمینه های پژوهشی و تحصیلی منفرد است و پرداختن به آن فرآیندی دشوار است. بنابراین، نیاز به رویکردهای جامع تری وجود دارد که بتواند تمام جنبه های مسأله را در نظر بگیرد.

با توجه به موارد فوق، هدف این پایان نامه پرداختن به این حلقه مفقوده با راه اندازی ابزارهای پشتیبانی همه جانبه نوآورانه است که تمام جنبه های مشکل و پویایی آنها را در نظر می گیرد. برای این منظور نوع جدیدی از مدل های انتقال و انتشار آلاینده های محلول و ابزار ارزیابی پایداری نوآورانه ای معرفی و ارزیابی می شود. شبیه‌سازی‌های *پویایی سیستم* برای این یکپارچه‌سازی به کار گرفته می شود چرا که این روش از قابلیت‌های ویژه ای در پردازش انواع مختلف داده‌ها و روابط متقابل بین زیرسیستم‌ها برای ایجاد یک رویکرد جامع‌تر برخوردار است. این کار تصویری واقعی‌تر و پویاتر از کل سیستم ارائه می‌دهد که پویایی مسأله را در چشم‌انداز چرخه حیات سیستم نمایان می سازد. ابزار جدید با برقراری ارتباط با مدیران سایت های آلوده و انجام آزمایش‌هایی برای تأیید کاربردی بودن ابزار در پروژه های واقعی توسعه یافته است. یک سایت آلوده به عنوان سایت اصلی در این پایان نامه انتخاب شد. این سایت یک کارخانه چوب بری متروکه در هیورتسبرگا (Hjortsberga)، در شهرستان آلوستا (Alvesta)، استان کرونوبرگ (Kronoberg)، در جنوب سوئد است. این کارخانه چوب بری از اوایل دهه 1940 تا اواخر دهه 1970 مشغول فعالیت بوده است و میراثی از خاک و آب های زیرزمینی آلوده با پنتاکلروفنل (PCP) به جا گذاشته است. خاک آلوده در محل قبلاً برداشته شده است، اما آلودگی در آب های زیرزمینی دریاچه مجاور را تهدید می کند. همچنین برای توسعه ابزار پایه ارزیابی پایداری، یک سایت آب زیرزمینی آلوده به فلزات سنگین در جنوب غربی ایران و یک سایت آلوده پتروشیمی در قزاقستان برای تست مدل حمل و نقل در مقیاس بزرگتری انتخاب شد. ارزیابی پویا از این سایت‌های آزمایشی نشان می‌دهد که پایداری چرخه حیات فرضی یک روش آلودگی زدایی ممکن است در طول زمان واقعاً مطلوب نباشد. همچنین، برخی از فناوری‌های پاکسازی آلودگی های زیست محیطی ممکن است پایداری بسیار پایینی را در ابتدای پروژه آلودگی زدایی نشان دهند، اما اثرات منفی کلی را سریع‌تر از حد انتظار جبران می‌کنند و پایداری چرخه عمر بالاتری را ارائه می‌دهند.

Populärvetenskaplig sammanfattning

Den industriella revolutionen och den ständigt ökande efterfrågan på kemiska produkter för olika typer av varor har efterlämnat miljontals förorenade jord- och grundvattenområden runt om i världen. Man uppskattar att det finns cirka tre miljoner potentiellt förorenade mark- och grundvattenområden i Europa. Att hantera detta stora antal förorenade områden kostar miljarder euro varje år och saneringen av dessa förväntas ta flera decennier i nuvarande takt. Olika länder har olika strategier och planer för att påskynda saneringsprocessen. I Sverige finns det cirka 80 000 potentiellt förorenade områden, varav cirka 8 000 är klassificerade i riskklass 1 eller 2 av Naturvårdsverket. Detta innebär att de kan medföra "mycket hög" eller "hög" risk för människors hälsa respektive miljön. Enligt "En giftfri miljö", som är ett av de sexton miljökvalitetsmålen i den svenska miljöpolitiken, måste alla dessa områden vara sanerade senast 2050. I nuvarande takt beräknas detta dock ta mycket längre tid (cirka 150 år). En orsak till denna låga takt är den höga komplexiteten och inneboende osäkerheten i jord och berg som orsakar hög hydrologisk och biogeokemisk heterogenitet och variabilitet. Ur teknisk synvinkel gör detta det svårt att besluta om vilken åtgärd som ska vidtas och hur, eftersom det är svårt att på ett tillförlitligt sätt uppskatta hur långt och hur länge föroreningsplymen kommer att spridas.

Kostnader, tidsåtgång och komplex hydrogeokemisk dynamik är dock inte de enda problemen i detta avseende. Den potentiella risken för folkhälsan om åtgärder vidtas för sent eller i otillräcklig omfattning orsakar ett socialt tryck på beslutsfattarna. Även om man vidtar åtgärder för att avhjälpa problemen är det inte nödvändigtvis fördelaktigt. Det kan ha en omvänd effekt på den lokala miljön, så att den totala miljöfördelen blir mindre än de oönskade effekterna (t ex koldioxidutsläpp och avfallsproduktion). Utöver dessa direkta frågor finns det indirekta aspekter som lägre markpriser i närheten av förorenade områden och minskat psykiskt välbefinnande hos boende. Följaktligen är detta ett multidimensionellt och tvärvetenskapligt problem med många intressenter.

För att hjälpa till med detta komplexa problem har flera beslutsstödsverktyg utvecklats. Dessa verktyg är antingen inriktade på problemets tekniska aspekter i form av modellering av föroreningstransport eller på förvaltningsmässiga aspekter i form av verktyg för hållbarhetsbedömning (dvs olika typer av ekonomiska, sociala eller miljömässiga konsekvensbedömningar och vanligare en kombination av dessa tre). Modeller för spridning och transport av föroreningar försöker helt enkelt bedöma den risk som är förknippad med föroreningen i fråga genom att beräkna hur långt föroreningsplymen kan sprida sig, i princip utan hänsyn till andra aspekter av problemet. Verktyg för hållbarhetsbedömning försöker å andra sidan beskriva hur hållbara åtgärder kommer att påverka hållbarheten (i form av ekonomiska, sociala och miljömässiga effekter), oavsett hur föroreningsplymen förändras i tid och rum. Modeller för transport av föroreningar och verktyg för hållbarhetsbedömning integreras sällan ordentligt för att fylla denna lucka, helt enkelt för att de fokuserar på olika uppgifter och inte tar hänsyn till vad beslutsfattarna verkligen behöver. Ett sådant problem går utanför enskilda discipliner och är svårt för beslutsfattarna att hantera utan tillförlitligt och öppet stöd. Det finns därför ett behov av mer holistiska metoder som kan beakta alla aspekter av problemet.

Mot bakgrund av ovanstående är syftet med denna avhandling att fylla denna lucka genom att ta initiativ till nya mångsidiga stödverktyg som beaktar alla aspekter av problemet och dess dynamik genom att integrera modellering av föroreningstransport med verktyg för hållbarhetsbedömning. För detta ändamål utvecklades och utvärderades en ny typ av transportmodell och verktyg för hållbarhetsbedömning. Systemanalytiska simuleringar användes för att integrera möjligheter att ta hänsyn till olika typer av data och samspelet mellan delsystemen för att ge ett mer holistiskt tillvägagångssätt. Detta ger en mer realistisk och dynamisk bild av hela saneringssystemet som beaktar fältdynamiken i ett livscykelperspektiv. Det nya verktyget utvecklades genom att kommunicera med platschefer och genomföra försök och tester för att verifiera verktygets tillämplighet. En förorenad plats valdes ut som huvudplats i denna avhandling för att utveckla modellen för transport av föroreningar och det slutliga verktyget. Platsen är en före detta sågverksanläggning i Hjortsberga, Alvesta kommun, Kronobergs län, södra Sverige. Sågverket var i drift från början av 1940-talet till slutet av 1970-talet och har lämnat ett arv av förorenad mark och grundvatten med pentaklorfenol (PCP). Förorenad jord på platsen har redan avlägsnats, men föroreningarna i grundvattnet hotar den närliggande Sjöatorpasjön. För att utveckla det grundläggande verktyget för hållbarhetsbedömning valdes också ett område med förorenat grundvatten av tungmetaller i sydvästra Iran och ett område med förorenade petrokemiska produkter i Kazakstan för att testa transportmodellen i större skala. Den dynamiska bedömningen av dessa försöksområden visar att den antagna livscykelhållbarheten för en saneringsteknik kanske inte är optimal över tiden. Vissa saneringstekniker kan också uppvisa en mycket låg hållbarhet i början av saneringsprojektet, men kompensera de övergripande negativa effekterna snabbare än väntat och ge högre hållbarhet under hela livscykeln.

Papers

Appended Papers

I. **Naseri-Rad, M.**, Berndtsson, R., Persson, K. M. & Nakagawa, K., 2020. INSIDE: An efficient guide for sustainable remediation practice in addressing contaminated soil and groundwater. *Science of the Total Environment*. 740, 139879.

II. **Naseri-Rad, M.**, Berndtsson, R., McKnight, U. S., Persson, M. & Persson, K. M., 2021. INSIDE-T: A Groundwater Contamination Transport Model for Enhancing Sustainable Remediation. *Sustainability (Switzerland)*. 13, 7596.

III. Radelyuk, I., **Naseri-Rad, M.**, Hashemi, H., Persson, M., Berndtsson, R., Yelubay, M. & Tussupova, K., 2021. Assessing data-scarce contaminated groundwater sites surrounding petrochemical industries. *Environmental Earth Sciences*. 80, 371.

IV. **Naseri-Rad, M.**, Berndtsson, R., McKnight, U. S., Aminifar, A. & Persson, K. M., 2022. DynSus: Dynamic Sustainability Assessment in Groundwater Remediation Practice. *Science of the Total Environment.* 832, 154992.

Author's contribution to appended papers

I. The author conducted the literature review, disseminated the survey questionnaires together with the fourth author, analyzed site and surveyed data, conducted the modeling, and prepared the original manuscript together with the second author. Reviewing and editing was done by all authors.

II. The author conducted the literature review, disseminated the survey questionnaires, analyzed investigated data from the site, initiated the modeling concept, conducted the modeling, and prepared the original manuscript mainly under supervision of the second and the third author. Reviewing and editing was done by all authors.

III. The author conceptualized and made a framework for the contaminant transport model and conducted the transport modeling together with the second author.

IV. The author developed the dynamic sustainability assessment tool. Then, in collaboration with the fourth author, the results were assessed. Finally, the author wrote the manuscript and revised it based on feedback from the co-authors.

Supporting publications

Journals

Kamali Maskooni, E., **Naseri-Rad, M**., Berndtsson, R. & Nakagawa, K., 2020. Use of heavy metal content and modified water quality index to assess groundwater quality in a semiarid area. *Water (Switzerland)*, 12, 4, 1115.

Naseri-Rad, M., 2020. To fight with contaminants through INSIDE, *VATTEN-Journal of Water Management and Research. 76, 50-51.*

Conference Proceedings

Naseri-Rad, M. & Berndtsson, R., 2019, Shortcomings in current practice of decision-making in contaminated site remediation, Proceedings of *the 9th International Conference on Environmental Pollution and Remediation, 5th World Congress on New Technologies (NewTech'19),* Lisbon, Portugal

Naseri-Rad, M. & Berndtsson, R., 2021, Decision Support Systems for Real! – Recognizing Sustainability Dynamics in environmental clean-up action., Proceedings of *the Lund University Research Conference - Knowledge for Sustainable Development,* Lund, Sweden

Naseri-Rad, M., 2022, Sustainability Dynamics in Contaminated Sites Remediation Practice, Proceedings of *the 8th Joint Nordic Meeting on Remediation of Contaminated Sites,* Oslo, Norway

Abbreviations

SA	sustainability assessment
LCA	Life-cycle assessment
MCDA	Multicriteria decision analysis
DST	decision support tool
SD	system dynamics
ANP	Analytic Network Process
DEMATEL	DEcision MAking Trial and Evaluation Laboratory
VBA	Visual Basic for Applications
RMSE	root mean square error
SGU	Swedish Geological Survey
CLDs	causal loop diagrams
MNA	monitored natural attenuation
P&T	pump and treat
PRB	permeable reactive barrier
Biorem	bioremediation
PCP	Pentachlorophenol
TPH	Total petroleum hydrocarbons
INSIDE	INfluence based deciSIon guiDE

1. Introduction

1.1. Dealing with land and water contamination

Soil, sediment, and groundwater pollution through various types of contaminants imposes an increasing risk to human health and the environment. Moreover, it restricts efforts to redevelop brownfield sites. The magnitude of this problem is alarmingly large. Heavy metal and metalloid contamination of topsoil only is estimated to affect more than 50% of the EU land surface (Jarsjö et al., 2020). In total, it is estimated that there are about three million potentially contaminated sites across Europe. In Sweden, there are some 80,000 potentially contaminated sites, according to the Swedish EPA (2008), of which about 8,000 sites are in risk class 1 or 2. This means that they represent ”very high” or “high” risk to human health or the environment, respectively. Remediation of this large number of sites is a challenging task (Rajput et al., 2022). It is not only expensive (Maskooni et al., 2020), but also laborious and time intensive (O’Connor and Hou, 2018). Moreover, performing invasive remedy measures in the unseen subsurface media is associated with high uncertainty in the overall performance. Since the aim of remediation practices in contaminated sites is environmental improvement, it may be assumed that this is a “sustainable” action. However, like other kinds of land management development, remediation is associated with extensive economic (Söderqvist et al., 2015), social (Norrman et al., 2020), and environmental (Lemming et al., 2010) impacts. The negative impacts may outweigh the benefits in many cases (Anderson et al., 2018). These issues have led to a new paradigm in the environmental clean-up (remediation) industry, which requires addressing all the potential side effects that a remediation measure might have on society (Hou, 2020). This has been interpreted as two similar movements known as “sustainable remediation” in Europe and “green remediation” in the US (Hou and Al-Tabbaa, 2014).

1.2. Sustainable remediation in practice

Considering the three piers of sustainability, which are environmental, economic, and social considerations, sustainable remediation aims at minimizing the risk of contaminants in the environment with least environmental, social, and economic impacts. Enabling sustainable practice, however, depends on numerous underlying decisions (Hou, 2020), which are not always transparent while involve multiple stakeholders in the decision making process (Lehigh et al., 2020) with different or even contradictory perspectives and interests (Norrman et al., 2020). In this context, sustainability assessment (SA) is a tool to support such decision-making through assessing environmental, social, and economic costs and benefits of remediation practices (Braun et al., 2021).

Life-cycle assessment (LCA), standardized by the ISO 14040 series (ISO 14040, 2006), is considered as a comprehensive SA tool in some cases; though its focus is mainly on quantifying environmental impacts. Inclusion of social and economic aspects to LCA is still unmature and there is no overall consensus on it (Søndergaard and Owsianiak, 2018). Moreover, LCA can be data and time intensive and not readily accessible for the large number of contaminated sites. SA tools based on multicriteria decision analysis (MCDA), on the other hand, reduce the cost and complexity of decision-making (Bardos et al., 2016), although they may lack robust unbiased input, which might lead to unreliable outputs.

It should be noted that both LCA and MCDA-based SA tools are used to ultimately assess environmental, and if applicable, social, and economic aspects of remediation projects. However, such assessment still fails to capture the temporal variability and subsurface dynamics in the field, which are the driving force of performance of any remediation action. Also, such SA tools fail to highlight key system feedbacks (due to nonlinear problem structures known to exist in contaminated land management). This may lead to non-robust results, as hydrological and biogeochemical variations at the site can have a great impact on the choice of remedial measure and its efficiency over time.

1.3. Aims and objectives

This thesis is an attempt to guide remediation practice to a more sustainable future as a general aim. Complex and multi-dimensional problems with long-lasting consequences must be solved in a transparent and comprehensive way. This, however, must not hinder considering real-world dynamics occurring through criteria and component changes in time. In view of this, the specific objectives of this work may be summarized as:

i. analyzing effects of criteria interactions in site remediation practice to suggest relevant improvements aiming at a holistic system thinking,

ii. developing a contaminant transport model to fit the SA framework through providing reliable insights of contaminant spread in time and space,

iii. integrating the contaminant transport modeling with the SA in a system dynamics framework, to enable a more quantitative assessment of sustainability indicators in time,

iv. conducting uncertainty analysis for better communication of the results, and

v. testing the methodology on real-world case studies to demonstrate its validity for improving the SA of remediation measures at contaminated sites.

1.4. Structure of this thesis

The present thesis is a compilation consisting of an extended summary of the research stages that is followed by four appended papers. The four papers address the mentioned objectives of the thesis as follows:

Paper I: (i), (iv), and (v)

Paper II: (ii), (iv), and (v)

Paper III: (ii), (iv), and (v)

Paper IV: (iii), (iv), and (v)

In **Paper I,** a novel SA tool that recognizes criteria interactions in remediation practice is provided. This tool is based on MCDA methods and could be used as a stand-alone decision support tool (DST). **Paper II** proposes an efficient contaminant transport model based on the analytic solution of the general transport equation. This new method is designed and developed with the aim of fitting in SA. In **Paper III** the developed contaminant transport model in **Paper II** is developed further by applying it to a significantly larger site but fewer investigated data points and in connection to a groundwater flow model based on MODFLOW. This is to test its reliability in application to various situations. Finally, **Paper IV** integrates the initiated SA tool and the contaminant transport model through system dynamics (SD) simulations to provide the targeted dynamic sustainability assessment tool to give a more reliable holistic view of the problem.

This summary continues with description of materials and methods used for developing the mentioned models and tools in the thesis. Then, description of case studies of which data and characteristics are used to validate the tools come in chapter 4. Chapter 5 is devoted to discussing the results of all simulations and support by the tools. These results lead to conclusions in chapter 6. Finally, limitations of the study and ways for improvement and going forward come in the last chapter of this thesis.

2. Theoretical Background

This chapter gives a theoretical background to the relevant issues around dynamicity in contaminated site remediation and the necessity of inclusion of contaminant transport modelling in SA to recognize such dynamics.

2.1. Dynamicity in remedial actions

The impact of hydrogeochemical heterogeneities and variations may be summarized in contaminant transport models (Locatelli et al., 2019) that exist for this purpose. However, these tools can further complicate the decision process, as they may be fragmented into sub-disciplines that introduce additional biases and prevent a holistic evaluation of the site remediation (Lemaire et al., 2021). Integration of these models with SA tools has generally not yet been practiced, mostly because these are of a different nature and with different aims compared to SA tools. Therefore, there is an urgent need for new modelling approaches that can quantitatively assess the sustainability of the remediation scenarios in a more integrated way (Onat et al., 2016). Such holistic view is of paramount importance in finding innovative, more efficient, and less harmful approaches and techniques for more sustainable actions in a life cycle perspective. The holistic approach can guide the site managers through providing insights for both technology development and site-specific actions by highlighting crucial points to focus on for overall improvement.

For example, assuming that public acceptability of a technology like bioremediation will be higher than an energy intensive technology like pump and treat, which is a common assumption in existing SA tools, might not be reasonable in all cases. At certain sites, the former may fail or take too long to reach the desired outcome, which makes it no longer a favorable option and the acceptability of the technology may differ. Another example could be seeing that spending X Euros on, e.g., energy efficiency of remediation alternative A may provide twice as much overall sustainability that spending X Euros on e.g., waste reduction of remediation alternative B may provide. Overall sustainability here may be defined as net environmental, economic, and social benefits of implementing a technology.

2.2. Need for an improved SA tool

Existing MCDA-based SA tools are largely assuming a hierarchical structure for decision problem and consider independence of decisions' criteria. These tools, in principle, consist of three or four criteria – environmental, economic, and social, together with or without technical criterion. These are then divided into several sub-criteria (so called sustainability indicators in SA practice) for each criterion, being affected only by other indicators in the criterion. This creates a hierarchy with pronounced boundaries between the criteria. Such structure does not follow often complicated structures of real-word problems and consequently prevents efficient holistic assessment. For example, how can one decide if a sustainability indicator such as *remediation time* belongs to environmental, social, economic, or technical category? And, in case of falling into any of these categories, *remediation time* can only affect the other indicators in its category. This is a condition that seems not probable in the field. All aspects will eventually be affected by time, in any case. A scheme of such structure together with a more dynamic one, that seems more realistic, is outlined in Fig. 1.

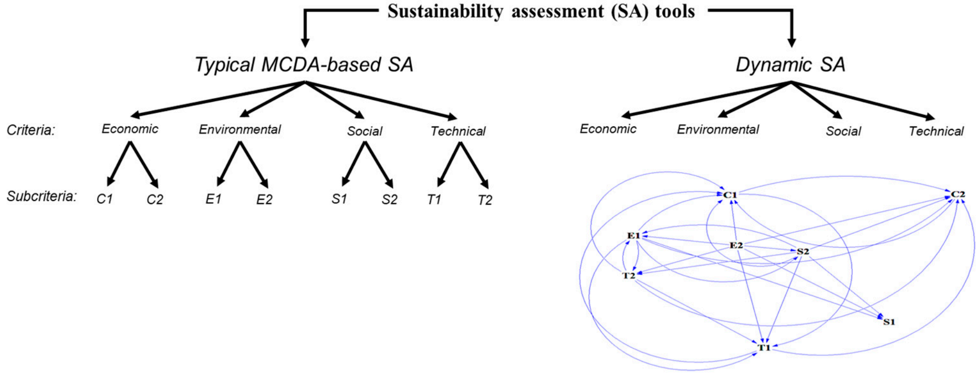


Fig. 1. Schematic of a traditional and improved MCDA-based SA tool.

Current MCDA-based SA methods help with constituting transparent and structured frameworks for decision-analysis problems (An et al., 2017, 2016; Li et al., 2018; Rosén et al., 2015). However, the linear interrelation among indicators and criteria independency assumption may be not fulfilled (Baykasoğlu et al., 2013) in more complex problems such as site remediation. A promising MCDA method that resolves these problems is the Analytic Network Process (ANP) (Saaty, 1996), in which, indicators in each criteria can affect each other and other criteria's indicators freely. In that sense there would be no boundary between criteria (environmental, economic, and social) and every indicator's relation with the other ones is recognized. Back to the example of *remediation time*, there would be no need to put this indicator in any of the criteria (environmental, economic, and social) as it can influence every other indicators with no restriction about the criteria that it falls into. However, ANP is hardly used in the remediation SA context, e.g., Promentilla et al. (2006) and Promentilla et al. (2008), because of its difficulty in application. This difficulty in the ANP comes from the need for many pairwise comparisons that might be time-consuming and too difficult to quantify in complex problems such as contaminated site remediation projects.

2.3. Contaminant transport modelling for SA

Numerical models for contaminant transport are often too detailed (Funk et al., 2017) to be applied for preliminary assessment of the large number of contaminated sites (McKnight et al., 2010), as they demand large amounts of investigation data (Locatelli et al., 2019). This leads to high cost that in any case, does not guarantee precise predictions (Zheng and Bennett, 2002). Simpler analytic and semi-analytic transport models, on the other hand, are less data intensive and, thus a better match in this regard (Harclerode et al., 2016). The common practice in the literature is the application of the advection-dispersion equation while considering a term for first order degradation based on Ogata, (1970), and Ogata and Banks, (1961).

BIOSCREEN (Newell et al., 1997) and BIOCHLOR (Aziz et al., 2002) are among simpler models that are commonly used to simulate solute transport with a first-order decay in 1D for dissolved hydrocarbons and chlorinated solvents, respectively. REMFuel (Falta et al., 2012), and REMChlor (Falta et al., 2007) are as well 1D models that allow simulation of enhanced plume remediation, but they are limited in spatial detail. An issue with these simpler models is that they might fail in considering proper values for site-specific parameters that must be assumed in the model. For that, inverse modeling is practiced as a prior step in the modeling process. Through inverse modeling (parameter estimation), the concentrations at specific points are given to the model. The model is then run to estimate other site specific parameters that fit best to the investigated data. Funk et al. (2017) developed the model HYDROSCAPE that provides both forward and inverse modeling modules, but its built-in parameter estimator module is limited to four data points.

These models, however, are not designed for integration with decision support system (DSS) platforms that, e.g., can consider the sustainability of the entire process. Such models must be simple and accessible enough for different stakeholders to apply and perceive the results.

3. Methods and Materials

3.1. Proposed SA in this thesis (Paper I)

3.1.1. Structure of the SA

The SA tool that is initiated in this thesis, is a three-step methodology. As Fig. 1 outlines, the criteria for sustainability assessment (also known as sustainability indicators) for evaluating remediation technologies are selected in the first step. Defining involved indicators is a fundamental step that structures the problem. Although there are some attempts to form a consensus for choosing these indicators, e.g., Braun et al., (2021), and Li et al., (2021) there is no single best choice for these (An et al., 2017). Thus, careful attention was paid to select these indicators based on detailed literature review, interviews with professionals (Naseri-Rad and Berndtsson, 2019), and discussions with different stakeholders. Finally, the three pillars of sustainability, i.e., social, economic, and environmental aspects, together with technical aspects were considered as main criteria. Then, eight sustainability indicators were selected based on these four categories. These eight sustainability indicators throughout this thesis, are: capital and operational costs, remediation time and efficiency, public acceptability, environmental impacts (emissions and waste generation), risk for secondary contamination (chemical or biological transformation of contaminants to more or equally harmful species), and human health.

In the second step, DEcision MAking Trial and Evaluation Laboratory (DEMATEL) method (Gabus and Fontela, 1972) defines the criteria interdependencies and assigns weights to them. This is done based on global considerations and not delimited to a particular contaminated site.

Finally, in the third step, ANP is used to prioritize different remediation technologies. This step is site-specific and follows remediation technologies for a contaminated site.

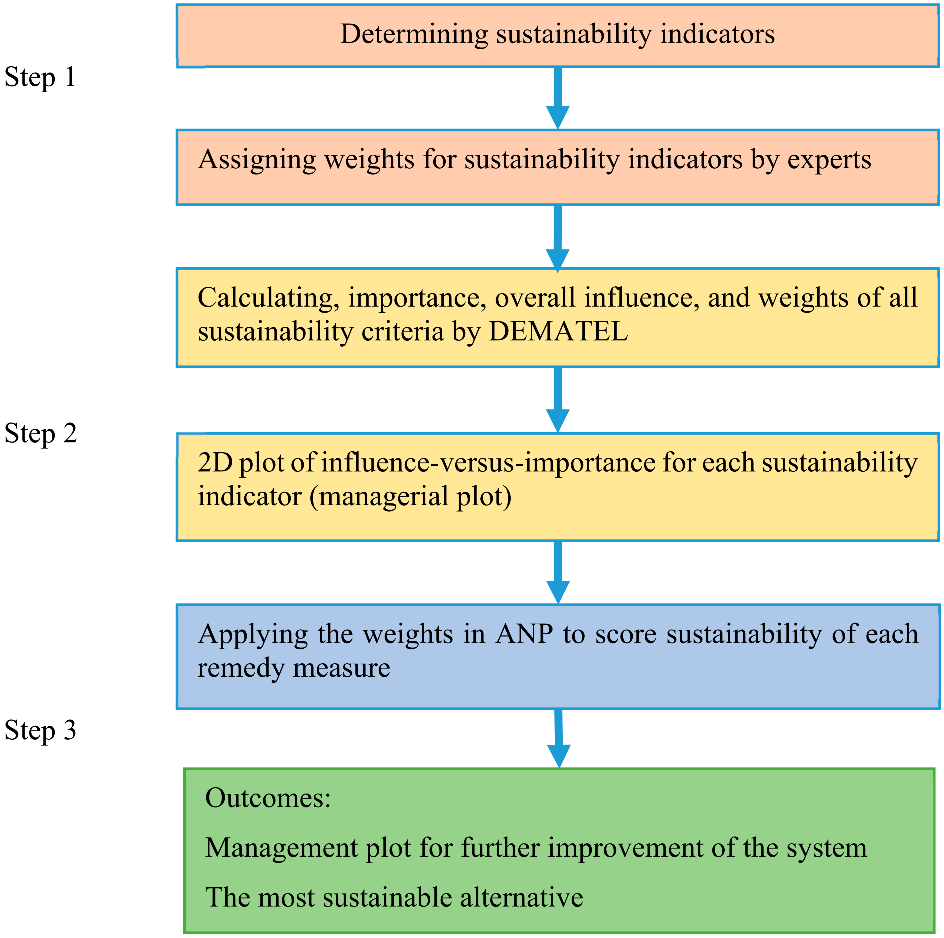


Fig. 2. Suggested SA approach for selecting the most sustainable technology and managerial approach for contaminated site remediation.

To feed the model in step 2 and 3, we applied surveying aiming at international experts regarding their opinion and quantification of the different criteria's importance and interdependencies. This was done through two questionnaires. *Questionnaire 1* included general queries with the aim of finding weights and interdependencies of criteria. *Questionnaire 2* focused on the actual case study with the aim of selecting remediation technology based on the weights from the first questionnaire.

3.1.2. Selection of sustainability indicators

Sustainable remediation can be defined differently but there is general consensus about its final purpose (Ridsdale and Noble, 2016), which is stated as balancing the desired and unwanted impacts of remediation actions in terms of the three most important aspects of sustainable development i.e., social, economic, and environmental aspects (Bond and Morrison-Saunders, 2011). Considering this final purpose, the eight criteria in Table 1 were chosen.

Table 1. Considered sustainability assessment criteria.

Aspect	Criterion	Reference	Abbreviation
Economic aspects	Capital cost	Hou *et al.* (2018)	Cap. Cost
	Operational cost	Hou *et al.* (2018)	Ope. Cost
Environmental aspects	Environmental impacts	Lemming *et al.* (2012)	Env. Imp.
	Risk for secondary contamination	Fan *et al.* (2019)	Sec. Con.
Technical aspects	Remediation time	Visentin *et al.* (2019)	Rem. Time
	Remediation efficiency	Visentin *et al.* (2019)	Rem. Effi.
Social aspects	Public acceptability	Hou *et al.* (2014)	Pub. Acc.
	Risk of exposure to humans	Hou *et al.* (2016)	Expo. Risk

3.1.3. DEMATEL for weighting the criteria and ANP for ranking remediation technologies

DEMATEL uses direct influence of each indicator on the other indicators to calculate overall interaction in the system. Thus, a questionnaire was sent to international experts, enquiring about the influence of each indicator on the others. Furthermore, the respondents were asked about the importance of each aspect and criterion separately. This enabled to check how these assigned weights fit the calculated weights by DEMATEL.

To cover both direct and indirect influences that the criteria have on each other, appropriate indicators need to be introduced. Defined as prominence indicator (t+) and relation indicator (t-), they are calculated using:

$$t_i{}^{+} = \sum_{j=1}^{n} t_{i,j} + \sum_{j=1}^{n} t_{j,i} \qquad (1)$$

$$t_i^- = \sum_{j=1}^{n} t_{i,j} - \sum_{j=1}^{n} t_{j,i} \qquad (2)$$

where $t_{i,j}$ shows the direct influence of the i-th criterion on the j-th criterion. t_i^+ is called prominence or importance of criteria i and t_i^- is called relation or influence of the criterion i on the other criteria.

In this study the DEMATEL is not used for prioritizing remediation techniques. It is instead used to calculate weights. Consequently, two more steps are necessary according to:

$$\omega_i = \sqrt{(t_i^+)^2 + (t_i^-)^2} \qquad (3)$$

where weights are normalized:

$$W_i = \frac{\omega_i}{\sum_{i=1}^{n} \omega_i} \qquad (4)$$

and W_i are the calculated criteria weights to be used in the decision-analysis process.

In step 3 (Fig. 1), the calculated weights are used as input to the ANP to calculate the overall score of each remediation method. The output of this step is interpreted as the most sustainable option for remediation according to the defined sustainability assessment framework.

Unlike most other MCDM methods that consider a hierarchical structure and independency of criteria and alternatives, ANP recognizes dependencies and influences of criteria. This makes ANP a pragmatic and beneficial tool to solve complex decision-analysis problems.

A typical entry of the super-matrix Wij is defined as:

$$W_{ij} = \begin{bmatrix} W_{i1}^{(j_1)} & W_{i1}^{(j_2)} & \dots & W_{i1}^{(j_{n_j})} \\ W_{i2}^{(j_1)} & W_{i2}^{(j_2)} & \dots & W_{i2}^{(j_{n_j})} \\ \dots & \dots & \dots & \dots \\ W_{in_i}^{(j_1)} & W_{in_i}^{(j_2)} & \dots & W_{in_i}^{(j_{n_j})} \end{bmatrix} \qquad (5)$$

Each column W_{ij} is a principal eigenvector of influence for the elements in the component of the network on the j-th component. By raising limiting powers on the weighted super matrix, global priorities are obtained as:

$$\lim_{n\to\infty} \boldsymbol{W}^n \qquad (6)$$

The above calculations were made in MATLAB® that was designed and checked for group decision making. However, the application of the proposed SA tool is not delimited to the four sustainability aspects and eight criteria associated to these. The method and the developed code can be used for any number of criteria and sub-criteria (indicators).

3.2. Proposed contaminant transport model for SA applications (Paper II & III)

Scoring process in the proposed SA tool can be substantially improved if stakeholders have a picture of what consequences each remedial action might have (representing performance outcomes in terms of contaminant concentrations for a potential decision). A new contaminant transport model is therefore developed here to bridge this gap. Figure 2 outlines the framework for this new model and its role within the SA tool methodology.

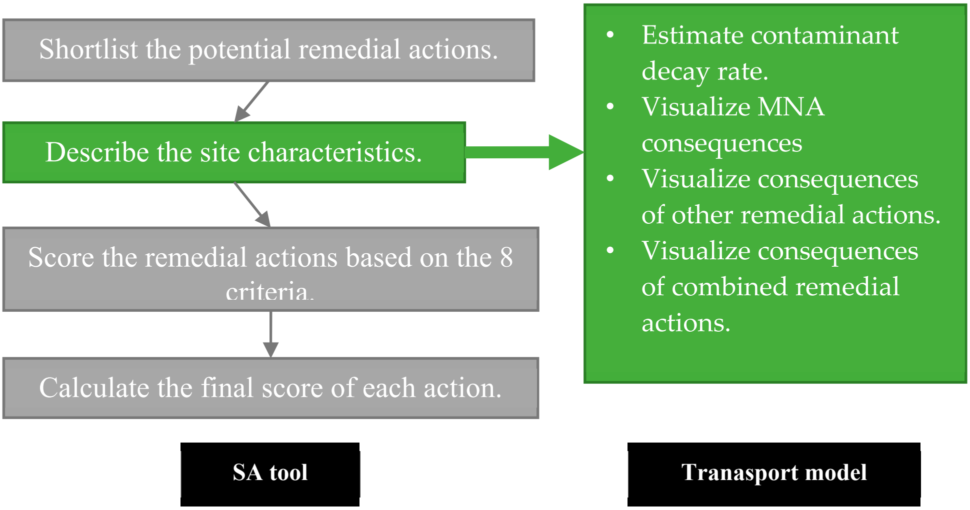


Fig 3. Framework of the contaminant transport model applied in this thesis (green boxes) as a part of the structure of the SA tool (grey boxes).

A participatory DST like the proposed SA tool in this thesis is envisioned to be readily applied by managers and stakeholders of various backgrounds. For this purpose, the transport model should be able to simulate the concentration change reliably, addressing the associated uncertainty. Therefore, this model is programmed in commonly used spreadsheets, and only one simple Visual Basic for Applications (VBA) Macro is used for developing it in Microsoft® Excel®. The

VBA Macro does parameter estimation in the first step. Parameter estimation may be defined as the determination of parameter values that govern the behaviour of a system, assuming that the mechanism of the process and the modelling outcomes are known. In the case of this thesis, parameter estimation includes solving the transport problem as many times as needed to minimize the model error. The error is the difference between measured and calculated values at observation points and times, which can be defined as mean absolute error or root mean square error (RMSE). Minimizing the error is done by changing involved parameters in the transport process in their ranges until the minimum difference between modelled and measured values is reached.

After inserting observed concentrations, hydraulic gradients, and locations of sampling points, a range for transport parameters is specified. The model then calculates the concentration at any point down-gradient of the source by modifying the parameters, according to their determined ranges, to minimize the error.

We consider the advective dispersive equation for solute transport that is based on partial differential equations of dispersion, developed for homogeneous and isotropic media where Darcy's law is valid:

$$D_L \frac{\partial^2 C}{\partial x^2} + D_T \frac{\partial^2 C}{\partial y^2} - v_x \frac{\partial C}{\partial x} = \frac{\partial C}{\partial t} \qquad (7)$$

where C (M/L3) is solute concentration, D_L (L^2/T) is longitudinal hydrodynamic dispersion, D_T (L^2/T) is transverse hydrodynamic dispersion, and v_x (L/T) is the average linear velocity.

We only give measured values of the exact location of the downstream points in terms of X and Y (which stand for longitudinal and transverse distance from the source – considering flow direction), contaminant concentration at source, and hydraulic gradient between any desired well and the source. Other required parameters will merely be the ranges of change in their values.

The proposed model is first applied to a case study in Sweden to illustrate the applicability in a real-world, environmental clean-up project. The model parameters used in the case study are taken either from field measurements by Swedish Geological Survey (SGU), which is the responsible organization for remediation of the site, or from relevant literature and technical reports with similar conditions. The aim is to perform an inverse modelling to estimate transport parameters, and based on that, performing a forward modelling to provide the decision-maker(s) with a reliable visualization of the potential consequences of a chosen remediation option.

The model is then applied to a site in Kazakhstan, in Paper III, to test its reliability for a data scarce area. Data scarcity is a common issues in handling contaminated sites (Locatelli et al., 2019) and risk assessment of contaminant spread (Maskooni et al., 2020) in most cases, especially in developing countries that have limited resources to spend on investigations. Such screening model can help in these situations with showing potential thread of a contaminant source to the downgradient regions. Groundwater flow modelling using MODFLOW is practiced in Paper III in parallel to the described contaminant transport model in this section both for confirming estimation of the in common parameters in both models (e.g., hydraulic conductivity, and flow rates), and for analysing groundwater flow direction and potential plume pathways that may govern the plume spread directions.

3.3. Improved understanding of site dynamics (Paper IV)

Due to the often-complex chemical, biological, and hydrogeological processes found at contaminated sites, because of e.g., soil heterogeneity, analysing the site-specific investigated data is necessity. This is due to the need to improve the understanding of the current state, key dynamics (change rate of variables) of the field conditions, and possibility for prediction.

For this reason, a K-means clustering method is applied – using the scikit-learn package (sklearn.cluster.KMeans) in Python – for categorizing the observation wells based on available time series for key observed hydrogeochemical variables. This is done to improve the understanding of the chemicals´ dynamic pattern over time and determine their variability. The two most popular types of clustering methods are partitioning clustering and hierarchical clustering. K-means clustering, where K represents the desired number of clusters, is a type of partitioning clustering where each cluster is defined by the centroid (or mean) of data points in the cluster. Moreover, a genetic algorithm-based machine learning method through Eureqa® Software was used to test the ability to predict concentrations spatially and temporally based on hydrogeochemical data form the site. Genetic algorithms are widely used in optimization problems and are applied here to find relationships between observed parameters and contaminant concentrations in groundwater at certain times and locations for prediction.

3.4. System dynamics approach (Paper IV)

System dynamics (SD) simulations is chosen as an integrative modelling method in this study due to its specific ability to systematically describe the relationship between system structure and behaviour. Integrating contaminant transport modelling with sustainability assessment, SD allows assessing the impact that temporal dynamics may have on acceptability of a remediation action.

SD is an interdisciplinary approach to represent complex systems by analysing their dynamic behaviour over time (Forrester and Senge, 1980). In other words, SD is a strategy for information processing, including information feedback (Ford, 2010) with the focus on the piecing together of (relevant) subsystems to give rise to a more transparent total complex system (McKnight and Finkel, 2013).

SD is especially suited for dealing with contaminated sites, since it can incorporate past remedial strategies that may have been undertaken to decrease the contamination levels and thus played a role in shaping the current situation found at a particular site (McKnight and Finkel, 2013). It permits both deterministic and probabilistic investigations (Lemaire et al., 2021) of the dynamic behaviour of a system, where causes and effects can change based on time-dependent boundaries of the system. Thus, SD provides a flexibility that is lacking in other methods, including increased speed of model development, ability to simulate interactions between model components, and better transparency resulting in improved confidence for all the stakeholders involved.

3.4.1. Building the SD model

Feedback is a crucial concept in the application of system dynamics simulation tools, as this is the primary mechanism often underlying the nonlinear behaviour that typically governs (natural) systems. To better explore and communicate the inherent feedback structure of a particular system, causal loop diagrams (CLDs) are commonly used (Sterman, 2000). A CLD consists of the governing and key supporting variables, which are connected by arrows to indicate their causal interrelationships. Each arrow is then assigned a positive (+) or negative (–) sign to indicate the direction of each interrelationship, i.e., how the dependent variable is expected to change when the independent variable alters. A positive link signals that when the independent variable increases, the dependent variable will increase too. This positive feedback relationship can lead to what is called reinforcing behaviour (or loops, when 3 or more variables are considered); such loops tend to drive uncontrolled (e.g., exponential) growth. In contrast, a negative link signals that an increase in a causal (independent) variable will result in a decrease in the dependent variable (effect), and results in balancing behaviour/loops; these loops are of critical importance in natural systems, as they provide the controls to limit (or balance) the growth. As a rule, to determine the behaviour of a loop, one must count the negative signs in the loop. Whether this is odd or even determines if the loop has balancing or reinforcing behaviour, respectively.

CLDs can thus be used to help identify the critical system variables and their feedback loops that may be governing the dynamic behaviour in a system under investigation (Ford, 2010), as well as ensure that policy or management decisions taken will have the desired effect (e.g., often the reduction or removal of unwanted reinforcing behaviour). In this way, CLDs can be used to either break down or build up complex systems (as a series of sub-systems) for enhanced transparency and communication purposes. According to recognized sustainability indicators (Naseri-Rad et al., 2020), a CLD for a generic remediation project is presented in Fig. 4.

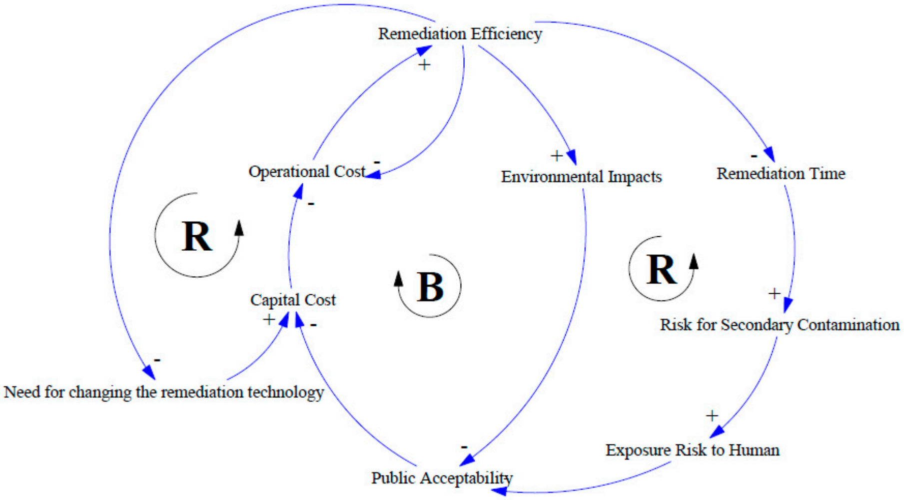


Fig. 4. Causal loop diagram of remediation practice, based on recognized sustainability indicators.

CLDs are typically used to support and enhance communication of the base model (and inherent assumptions in its derivation), as is done here, or can be used to explore the current understanding of a system more qualitatively. This can form the basis for creating a quantitative simulation model (or support efforts for data generation to enable this).

Another central concept in developing SD models is the identification and representation of the system’s “stocks and flows”. Stocks are used to represent accumulations in the system and their change over time. A stock thus gives insight into the current state of key modelled variables, as well as their dynamicity at any point during the simulation, and as such, can provide information to support the decision-making (Sterman, 2000). Flows, on the other hand, are the rates at which a stock may be decreasing or increasing (representing the outcome of a series of linear and/or nonlinear processes). From a mathematical perspective, an SD model is composed of coupled first-order integral equations, having the form (Forrester, 1961; Sterman, 2000):

$$Stock\ (t) = \int_{t_0}^{t} [Inflow(t) - Outflow(t)]dt + Stock(t_0) \qquad (8)$$

where Inflow(t) and Outflow(t) represent inflows and outflows at any time t between the initial time t_0 and t, respectively. Stock(t) and Stock(t_0) are the state of the system (the amount of the variable of interest accumulating in the stock) at times t and t_0, respectively.

The target parameter of the simulation – sustainability – is taken as the parameter in the Stock. Sustainability of any remediation action can then be measured as the change in the stock. Inflows to and outflows from the Stock are factors responsible for either increasing or decreasing the sustainability, respectively. These factors are comprised of the 8 sustainability indicators and their weights. A stock-and-flow diagram, highlighting the interactions and influential factors, is shown in Fig. 2.

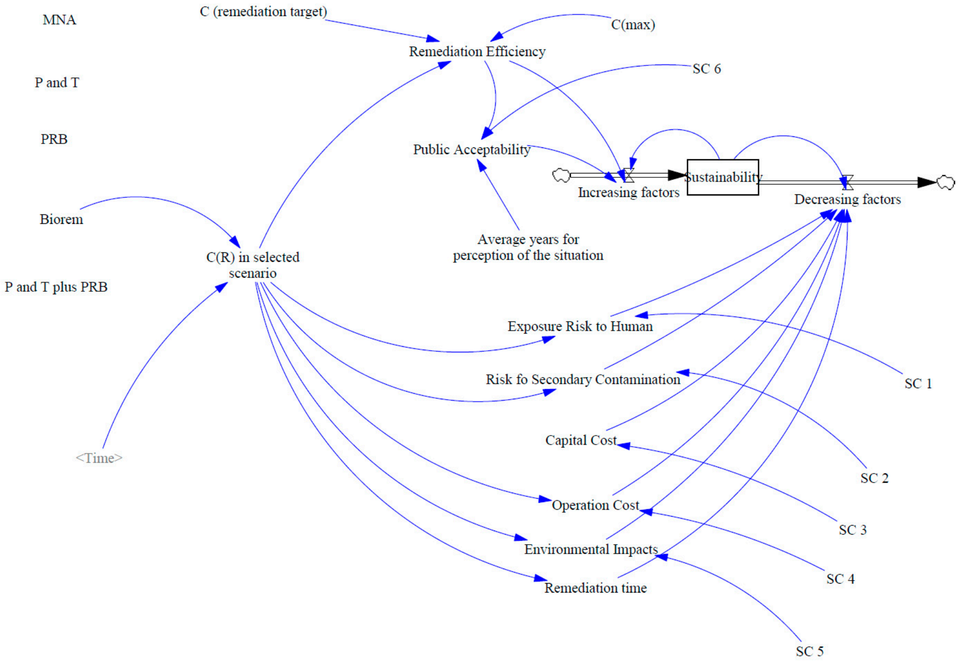


Fig. 5. Stock-and-flow diagram of the SD simulation model, combining recognized sustainability indicators with key contaminant variables.

The first step in the application of the SD model is to choose from the five available remediation options that are chosen for the case study (Paper IV). In Fig. 5, bioremediation has been chosen, and is thus connected to the variable it should influence, which is concentration at the recipient (C(R) in selected scenario). As it will be explained further in section 3, considered remediation technologies for the site in question include: monitored natural attenuation (MNA), pump and treat (P&T), permeable reactive barrier (PRB), bioremediation (Biorem), and combination of P&T and PRB systems (P&T + PRB). C(R) is already estimated through the contaminant transport model (Paper II) and is imported here for the case of each remediation alternative.

C(R) in the selected scenario can be defined as ”remediation efficiency” as they both imply the same measure. Thus, remediation efficiency is calculated as the portion of concentration that is removed by the selected remediation scenario: [C(max)-C(R) in selected scenario]/C(max). C(max) is the initial contaminant concentration at the recipient at the beginning of all remediation scenarios. C(max) is put 1790 µg/l as the concentration of contaminant at the end of 2020 and before performing remedial actions at the case study (Paper II). Remediation efficiency is however set to 0 for the time before 2020, as there was no remediation option in place, and 1 for the time the remediation target concentration (in our case study, 100 µg/L) is reached.

Remediation efficiency is the most important objective measure that affects all the eight criteria and might even impact the choice of remediation technology. According to the CLD in Fig. 4, it affects all eight criteria and even the choice of remediation technology, but not the capital cost. The capital cost represents the total budget needed to get a remediation technology up and running and is basically fixed. If the remediation efficiency should be deemed as not satisfactory at some point, it may necessitate changing the remediation technology, which may directly change the capital cost as demonstrated by the factor Need for changing the remediation technology in the CLD (see Fig. 4).

However, remediation efficiency is not the only variable that affects all criteria. Each technology has impacts on every criterion to some extent. For example, regardless of how efficient a P&T scenario may be, it might have a lower public acceptability because of its higher environmental impact and exposure risk to humans (as it requires the contamination being pumped up to the ground). These are subjective impacts and their ability to affect the system is modeled here and denoted by SC1 to SC6 (stands for scenario coefficients). These scenario coefficients are basically weighting factors that may be assigned by experts and may differ in a case-specific manner. For this, a questionnaire was sent out and asked remediation experts to score coefficients for each remediation technology with regards to other alternatives (Naseri-Rad et al., 2021). The only criteria with no scenario coefficient assigned are remediation efficiency and remediation time as these are estimated by the contaminant transport model, and thus do not need to be considered by stakeholders, which is currently a common practice found in existing SA tools (e.g., Hou, 2020; Hou et al., 2018b; Li et al., 2018; Onwubuya et al., 2009; Rosén et al., 2015).

Also, it is a reasonable assumption to consider that increasing contaminant concentrations at the recipient (C(R) in selected scenario) will result in increasing Exposure Risk to Human, increased Risk for Secondary Contamination, increased Operational Cost and increased Environmental Impacts (due to higher need for action to increase efficiency). These four criteria are therefore assumed to change over the life cycle of a project proportional to the relative concentration at the recipient (C(R) in selected scenario/C(max)) multiplied by the scenario coefficients that experts assigned for each technology. Opposite to these criteria, as contaminant concentrations at the recipient (C(R) in selected scenario) increase, Remediation Efficiency and Public Acceptability decreases. These factors are thus assumed to change inversely proportional to the normalized relative concentration at the recipient ([C(max)-C(R) in selected scenario]/C(max)).

However, it may take some time after contaminant concentrations reach a certain level before it may change Public Acceptability which is accounted for in the factor Average years for perception of the situation. This is assumed to be two years; meaning that it would take two years after contamination concentrations reach a certain limit that the public/local residents would recognize the change and may react accordingly. For example, it will probably take some time after concentration levels reach an acceptable level for local land prices to rise again due to no more contamination at the site. In terms of the remaining criteria, Capital Cost is not dependent on the efficiency, and may change if the remediation technology alters; Remediation Time represents only the time period that the contaminant concentration at the recipient has not reached the target remediation concentration. Thus, Remediation Efficiency and Public Acceptability are Increasing factors while the other criteria represent Deceasing factors in measuring the sustainability of a remediation practice (as shown in Fig. 2).

4. Case Studies

4.1. Heavy metals in Gachsaran, Iran (Paper I)

To apply the proposed SA methodology to a real-world problem, the Emamzade-Jafar Aquifer in Gachsaran region in southwestern Iran is used as a case study (Fig. 6). This is a partly contaminated aquifer with significant data scarcity. Although lack of reliable data is very common for many sites (Locatelli et al., 2019) in most countries, it causes more problems in developing countries where the lack of funds does not allow for detailed investigations. So, decision makers need to make fundamental decisions based on very limited data. Often, many contaminated sites are left with no remediation.

Except for agricultural contaminated sites (Hou et al., 2018), most contaminated sites are quite small and situated on top of one large aquifer. In Gachsaran, contaminant concentration data is to a major extent lacking in a way that prohibits identification of pollutant sources. Samplings have only been performed at a few points.

The aquifer is located in a semiarid region with groundwater flow direction from north-west to south-east. According to the Iran Water Resources Management Company (IWRMC, 2019) the groundwater table depth within the region varies from about 20 to 80 m below ground surface in the southern and northern parts, respectively. The geologic media is composed of course material mixed with clay in the northern parts, mainly sandy clayey loam in the central parts, and finer material like silt and clay in the southern parts.

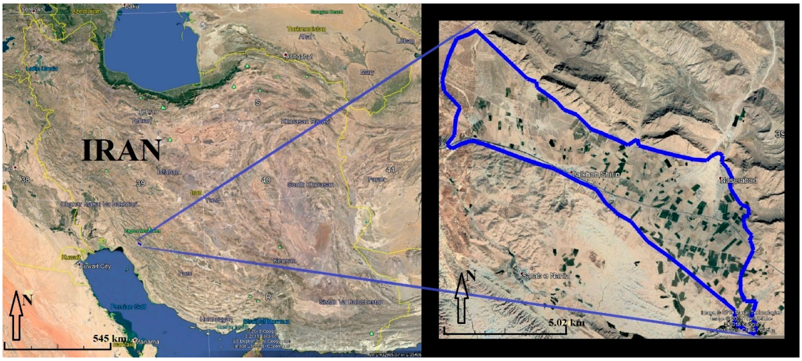


Fig. 6. Experimental study area, Emamzade-Jafar Aquifer in Gachsaran region in south-western Iran.

Sampling data show that especially concentrations of three heavy metals, selenium, cadmium, and antimony, are exceeding permissible levels with about 1.5, 4, and 10 times the permissible limits for drinking water use, respectively.

4.2. Pentachlorophenol (PCP) in a former sawmill in Hjortsberga, Sweden (Paper II & IV)

Chlorophenols were used in Sweden until 1978 for treating wood as fungicide during storage and transport. This is source of contamination at a former sawmill plant in Hjortsberga, Alvesta Municipality, Kronoberg County, southern Sweden (Fig. 7). Being in operation from the early 1940s to the late 1970s, the sawmill plant has left very serious contamination in soil and groundwater with pentachlorophenol (PCP), a branch of chlorophenols. The contamination in groundwater is threatening the nearby Lake Sjöatorpasjön, already hindering its use for recreational purposes and swimming. There are some farming activities in place surrounding the lake, too.

In 2013 all unsaturated contaminated soil was removed from the site with an excavator but the PCP concentration in groundwater is still well above safe limits.

Figure. 7. Location of the former sawmill plant, and sampling wells (all dots). Red dots show wells from which data are used in this study.

Geologic media

The typical stratigraphy in the area is bedrock covered by till (Axelsson and Håkansson, 2012). The deposits at Hjortsberga are described as “complex and heterogeneous” (Nord, 2019) and consist of coarse-grained glaciofluvial sediments, tills with different grain size, clay, and peat (Fig. 8). Commonly, the depth to bedrock is less than 5 m in the area, therefore, the surface topography may reflect the bedrock (Johansson, 2020). The composition of the till in the region is mostly sandy-silty (Johansson, 2006). The bedrock in Hjortsberga is of crystalline character with water-bearing fractures in a north-northwest to south-southeast and south-southwest to north-northeast direction (Johansson, 2006).

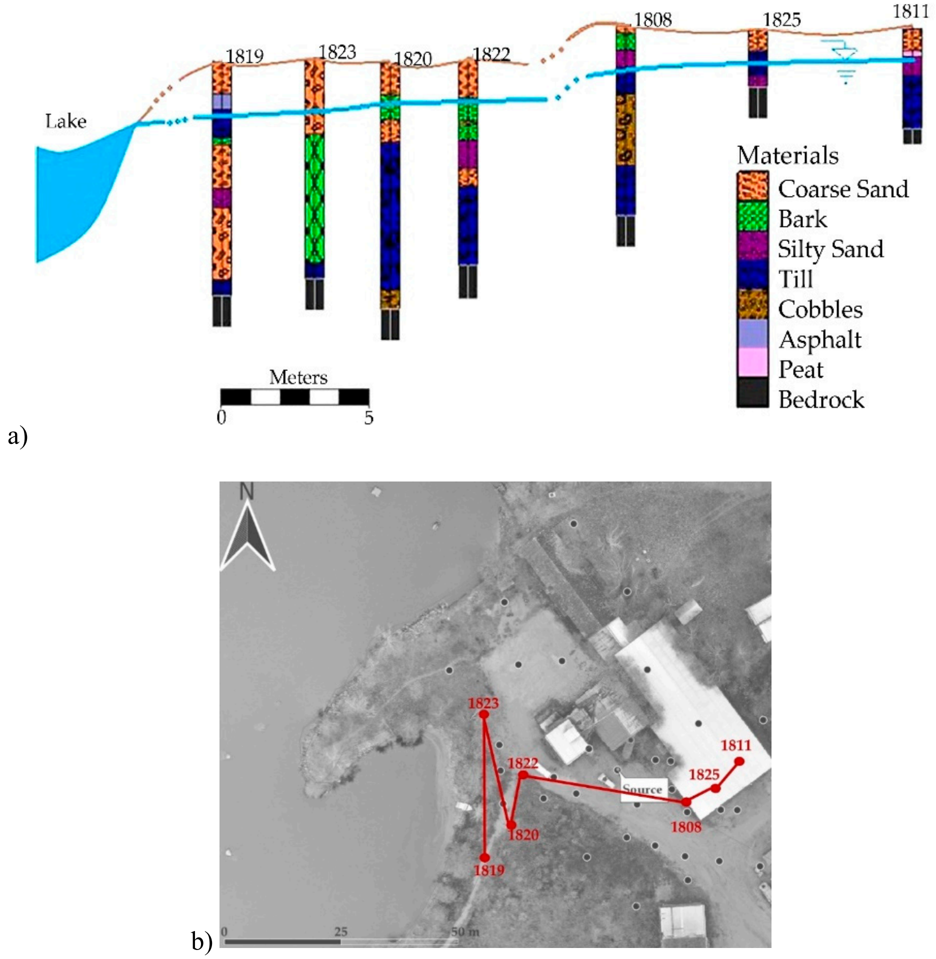


Figure. 8. a) Topography and geologic materials, and b) plan view location of selected boreholes at the field site (m).

Contaminant characteristics

Mobility of PCP is highly dependent on solution pH (Liu et al., 2019). Hurst et al. (1997) showed that PCP solubility at pH 4.2 is 13.2 mg/L and at pH 7.65 it is 1,465 mg/L (Hurst et al., 1997). Autochthonous microbes can remove low level PCP (<1.0 mg/L) to approach if not reach the regulatory standard of 0.001 mg/L with the addition of oxygen, with or without nutrient amendments (Schmidt et al., 1999). Although PCP in groundwater may be in non-aqueous phase liquids (NAPL) form as well (Rao et al., 2017), the form of contamination that is assessed here is the soluble form. This was as well observed in the field. Figure 9 shows a conceptual model for this.

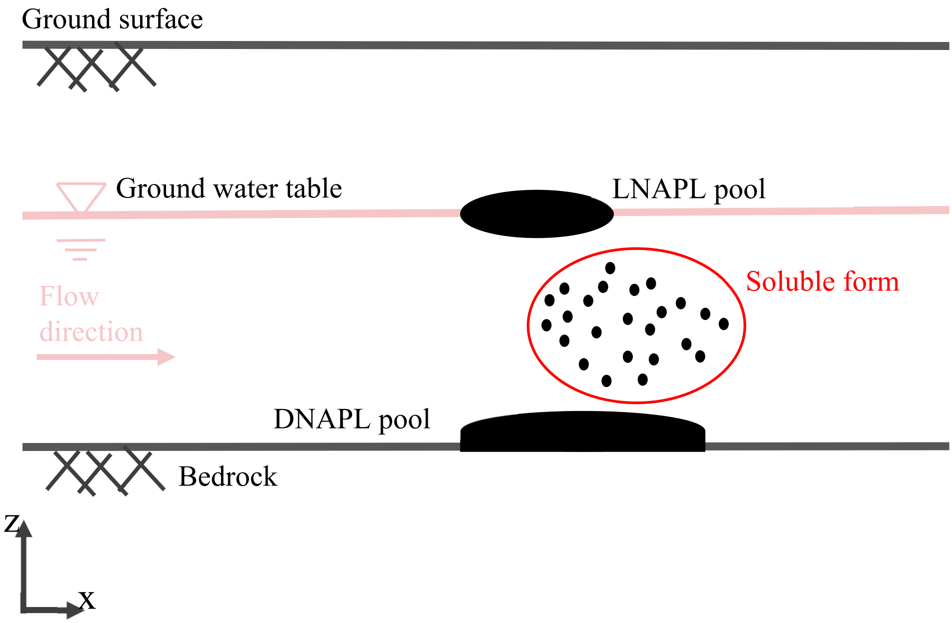


Figure 9. Conceptual model of PCP transport in subsurface and its different forms: dense NAPL, light NAPL, and soluble in water.

4.3. Total petroleum hydrocarbons (TPH) discharged from oil refineries in Kazakhstan (Paper III)

The source of potential contamination in this case study is a recipient pond “Sarymsaq”, where wastewater from several local petrochemical refineries is discharged. Even after primary treatment at the plants, it is difficult to remove hydrocarbons from the wastewater (Bruno et al., 2020). Only the sum of total petroleum hydrocarbons (TPH) is monitored at the site, without an assessment of the constituent potentially toxic chemical compounds.

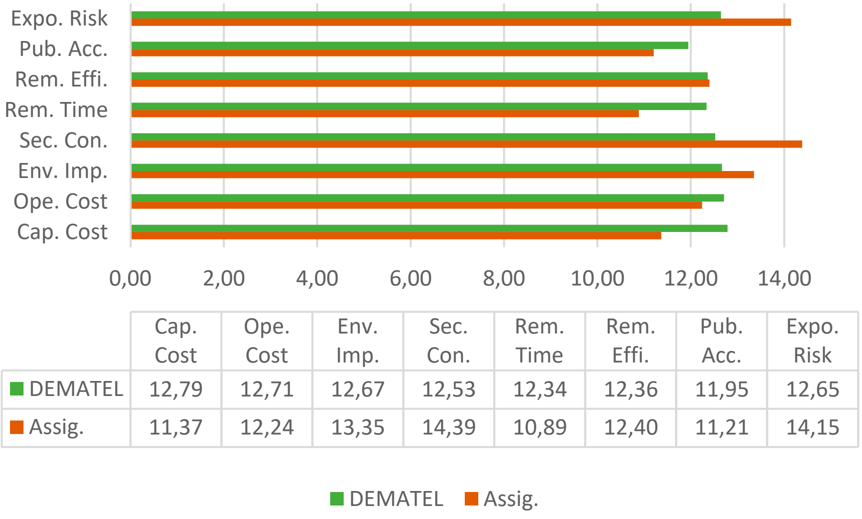
The hydrogeological cross-section is mainly represented by i) formation of Upper-Quaternary deposits of the first supra flood plain terrace, 4–5 km wide, ii) water-bearing sediments consist of quartz–feldspar sands, and iii) the top layer which is composed of sandy loam and loam, that at the bottom layer is composed of gravel and pebbles. The groundwater in the aquifer has a free surface. Aquifer thickness varies from 2 to 7 m in the northern and north-western parts of the area, and it increases in a south-easterly direction to 80 m. Water-bearing sediments consist of quartz–feldspar and micaceous sands. Groundwater depth is 2–28 m from the surface.

5. Results and Discussion

5.1. Insights provided by the proposed SA tool

INfluence based deciSIon guiDE (INSIDE) is developed in this thesis as the proposed novel SA tool that recognises criteria interconnection at the contaminated sites remediation practice. INSIDE aims at helping in real-world complex situations when there is no clear understanding of either problem structure or best solution. INSIDE further unveils realistic non-hierarchical interrelationships among decision criteria in groundwater remediation practice.

DEMATEL used the 51 interview results to calculate criteria weights, through Eqn. (3) and (4). Figure 10 shows a comparison between the calculated average weights by DEMATEL and directly assigned weights to the criteria by the interviewees. As the figure shows, there is a difference between DEMATEL results, and the weights directly assigned by the interviewees. Also, the weights differ between criteria. To evaluate these differences, an ANOVA analysis is performed.



	Cap. Cost	Ope. Cost	Env. Imp.	Sec. Con.	Rem. Time	Rem. Effi.	Pub. Acc.	Expo. Risk
🟩 DEMATEL	12,79	12,71	12,67	12,53	12,34	12,36	11,95	12,65
🟧 Assig.	11,37	12,24	13,35	14,39	10,89	12,40	11,21	14,15

Fig. 10. Assigned and calculated weights in percent based on respondents' opinions for each criterion.

The results show that the difference between DEMATEL calculated and assigned weights is not significant for any of the criteria (P-value=0.29>>0.05, Fig. 11). However, the difference between subjectively assigned weights is significant for the eight criteria: P-value=$6\times10^{-5} << 0.05$, (Fig. 12).

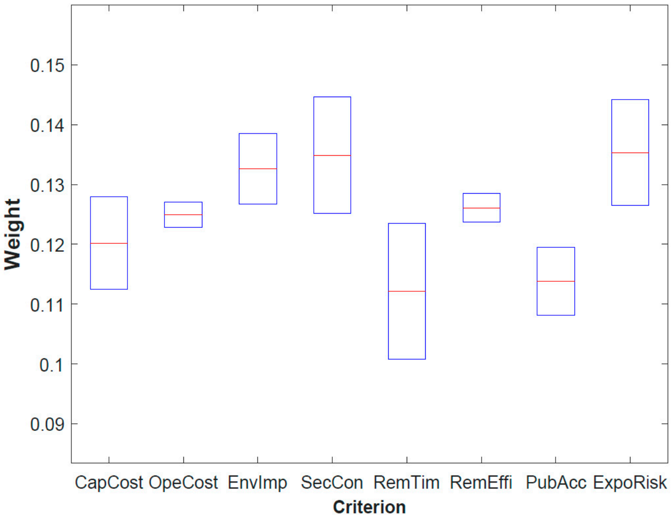


Fig. 11. Boxplots of ANOVA difference between DEMATEL calculated and subjectively assigned weights for each criterion. P-value from ANOVA equals 0.29.

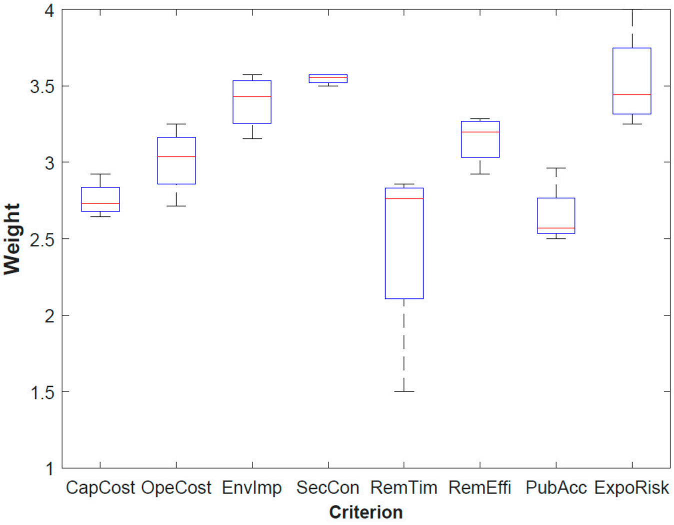


Fig. 12. Boxplots of ANOVA difference for subjectively assigned weights of each criterion. P-value from ANOVA equals 6×10^{-5}.

Moreover, DEMATEL enables to obtain a Network Relation Map (NRM) for the remediation practice. In the NRM each arrow shows a significant influence from the criterion where it originated, on the criterion where it ends (Fig. 13).

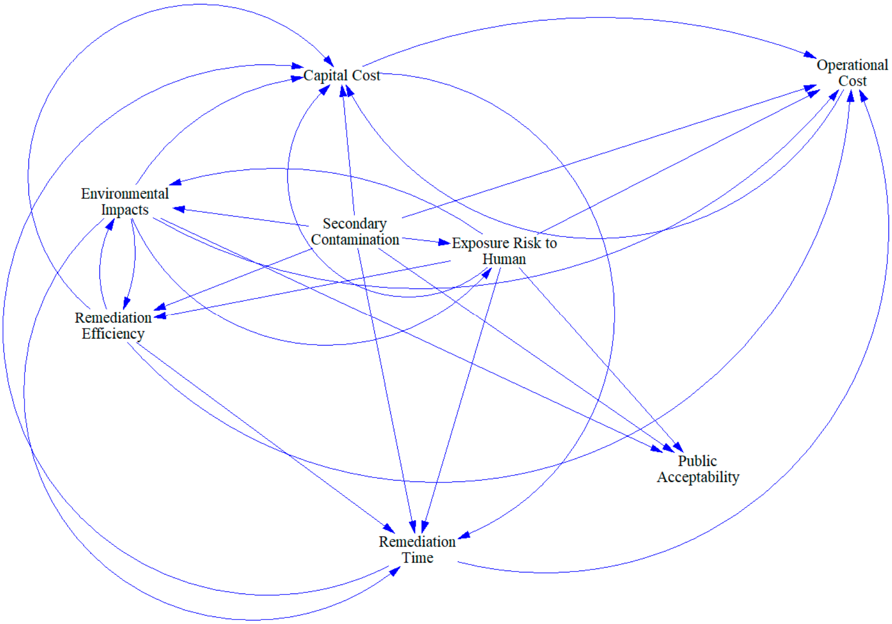


Fig. 13. NRM for the remediation system based on the respondents´ views.

Finally in INSIDE, the aim is to apply the calculated weights to decide about handling the contamination problem in the case study. The ANP prioritizes the remediation techniques at this stage based on the criteria interaction from DEMATEL. In total, 14 experts who were site managers, consultants, and university staff with experience in actual site remediation, were asked at this stage to give their opinions on scores to different remediation alternatives for each criterion.

As Fig. 14 shows, the best alternatives are *pump and treat* and *monitored natural attenuation* with close scores.

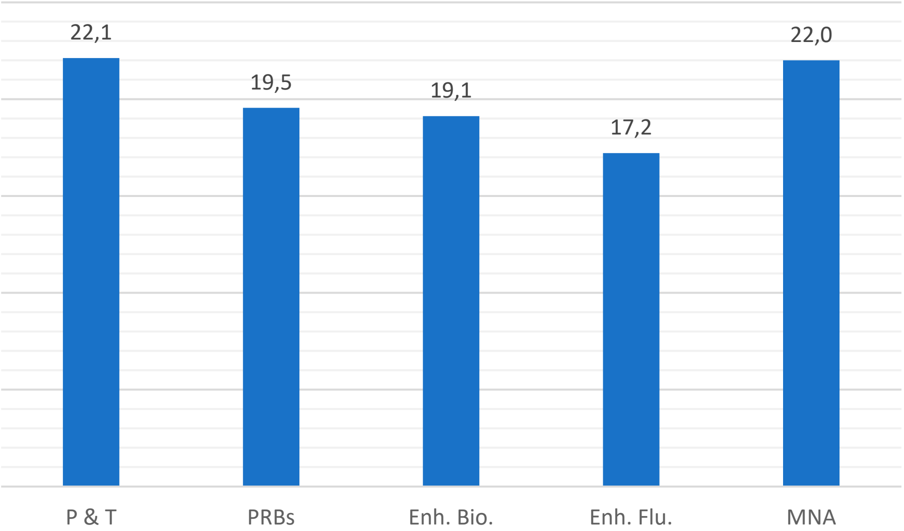


Fig 14. Output from the INSIDE approach for step 3, showing overall final scores for the five remediation alternatives (%).

Although INSIDE helps with structuring the problem and providing a transparent framework of the decision-making problem, it does not consider chemical variabilities and contamination spread in time. Such dynamics play an important role in the performance of any selected remedy measure and must be considered in further steps. For that, INSIDE-T was developed in this thesis (Paper II) and implemented on the Hjortsberga former sawmill in south Sweden as a case study, to show how a suitable contaminant transport model can help in addressing the mentioned issue. Hjortsberga was chosen as it is well investigated and under continuous monitoring and undergoing pilot remediations. Thus, there is sufficient investigation data for running a contaminant transport model. However, this is a quite small site with a specific contamination type. To ensure reliability of the contaminant transport model (INSIDE-T), it is applied to a significantly different site, both in size and characteristics. This is addressed in Paper III.

5.2. Insights provided by the contaminant transport modelling approach

The transport model, developed in this thesis, is named INSIDE-T for easy reference. INSIDE-T uses conservative assumptions and simplifications to give an estimate of contaminant spread, following inverse and forward modeling for investigation data. These estimations may be then used for scoring sustainability of each remedy scenario using the pre-assigned indicators' weights in INSIDE. The overall simple structure of INSIDE-T enables stakeholders to test different scenarios and quantify their sustainability score, regardless of their background and expertise.

As the main outcome of running parameter estimation (inverse modelling) in INSIDE-T, descriptive statistics of final transport parameters are shown in Table 2.

Table 2. Ranges of final transport parameters, distributions, and standard deviation.

Parameter	T	b	K	n_e	α_L	α_T	ρ_b	K_{oc}	f_{oc}
Unit	m	m	m/d	-	m	m	kg/L	L/ kg	-
Taken from	FM	FM*	FM	FM	Lit**	Lit	FM	Lit	Lit
Min	5	3	0.04	0.25	1	$\alpha_L/20$	1.9	398	0.0002
Max	65	5	40	0.35	30	$\alpha_L/6$	2.4	19953	0.02
1st quartile	9.00	3.00	4.00	0.30	26.00	2.60	2.17	398.00	0.0034
Median	9.09	3.00	4.00	0.32	27.68	2.77	2.20	398.47	0.0103
3rd quartile	10.52	3.03	4.60	0.35	28.00	2.80	2.20	399.96	0.0187
St. dev.	0.68	0.31	0.46	0.02	0.94	0.56	0.10	0.89	0.0074

* Field measurements (FM)
** Literature (Lit)

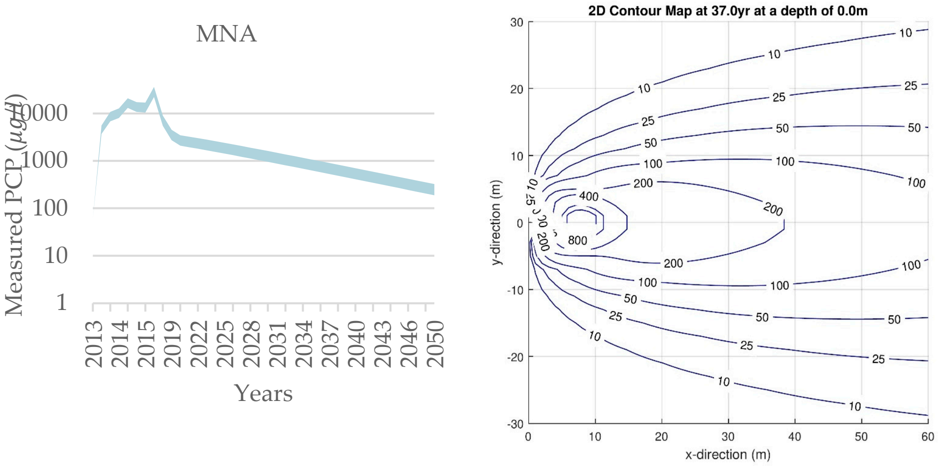
Median parameter values may be used for simulating the contamination transport in the time span of interest (forward modelling). However, to consider spatial and temporal variability of these parameters (McKnight and Finkel, 2013), especially regarding the needed long-term spans of the study simulations, and due to our limited knowledge of measurement accuracy and errors, the need to deal with the inherent uncertainty in parameter values is great. Thus, 1st and 3rd quartile values for all transport parameters were used to show the results in terms of most probable outcomes.

The shortest distance from the source to the recipient is 60 m along the straight source-recipient line with a 2 m distance from this line (x = 60 m, y = 2 m).

5.2.1. Assessing MNA as a remedial option

For forward modelling of contaminant transport, a PCP decay rate at the source needs to be estimated. Mass flux calculation was used to perform this estimation and the most conservative result was 100 years as contaminant source lifetime.

Figure 15a depicts the uncertainty in model output at the recipient (x = 60 m, y = 2 m) from 2013 to 2050 based on source - pathway – recipient approach. However, the model can be used together with a software that is capable of visualization of the plume in 2D. The inverse modelling results may give input to such a software and result in contours of iso-concentration simulated plume. HYDROSCAPE (Funk et al., 2017) was used here for this purpose that is based on analytical solutions for contaminant transport and fed with parameter values. Results of this application are shown in Fig. 15b.



a) b)

Figure 15. a) Simulation result for monitored natural attenuation (MNA) over a 37-year period in logarithmic scale, b) iso-concentration simulated plume lines, made using HYDROSCAPE, for spatial visualization of the plume (unit: μg/L).

Site managers at the Geological Survey of Sweden (SGU) are looking for reaching a contaminant concentration at the recipient corresponding to about 100 µg/L. As the model results show, and accounting for uncertainty, this condition might not be reached merely through natural attenuation in the time span of interest.

5.2.2. Assessing alternative remedial scenarios

A shortlist of remedial methods for the site includes P&T, PRB, bioremediation, and a combination of P&T and PRB. These alternatives are designated as scenarios 2 to 5, respectively. Figure 16 shows how these alternatives are likely to perform at the recipient, considering associated uncertainty.

As Fig. 16 illustrates, although we may reach lower concentrations quite early by performing P&T, the long-term performance of this technology might not be desirable.

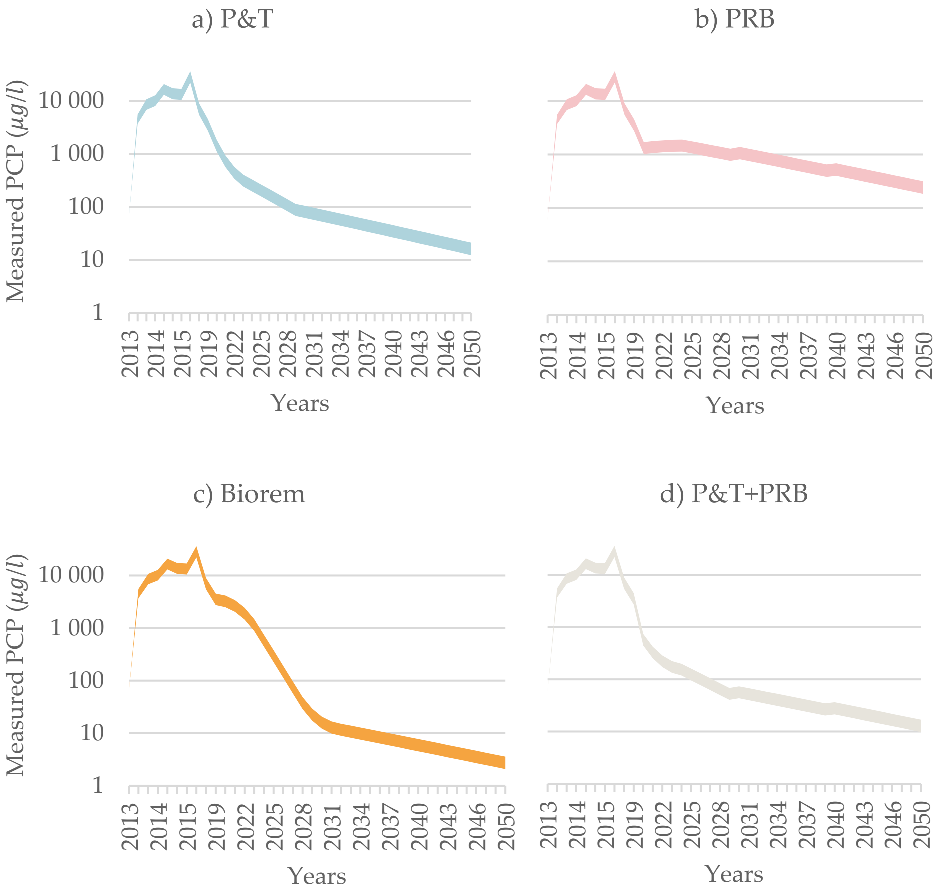


Fig. 16. Performance of different scenarios at the recipient in different years, considering associated uncertainty, for a) P&T, b) PRB, c) Biorem., and d) P&T+PRB. Concentrations are shown in logarithmic scale.

Application of PRB does not result in a significant decrease in recipient concentration. Bioremediation, on the other hand may reach the treatment target by 2026-2027 according to the figure, but high uncertainty in this method together with the model uncertainty may hinder its reliability.

The last scenario considered here is a combination of two previously simulated remediation techniques, P&T at the source and placing a PRB 35 m downstream of the source. Figure 16d illustrates the performance for this combination. High costs may apply in such combinations, which must be considered in the decision-making process.

It should be highlighted that the simulation results are associated with uncertainty and can be used to give a first impression of what may be expected in terms of performance capability for different remediation strategies. Cost and other uncertainties associated with the remedial measures need to be estimated. Here, a linkage between INSIDE-T and INSIDE may come into play to assist site managers considering other aspects.

The results of applying the proposed transport model in the new case study in Paper III together with MODFLOW for groundwater flow modeling were promising as well. The range of hydraulic conductivity and hydraulic head matched observations. Moreover, longitudinal, and transverse dynamic dispersivity together with plume width were considered as the most sensitive parameters. This was in line with the results in Paper II. Eventually, Paper III concluded that the contamination in question may migrate up to 5 km downgradient of the source.

5.3. Statistical methods to show the site dynamics

5.3.1. Clustering observation wells

For the case study in Paper IV, the results of the clustering by the k-means method for all observation wells and based on all chemical parameters, are illustrated in Fig. 17. A small noise of 1 m was implemented to avoid direct overlapping of the colour-assigned categorization for different time steps. Dots that are close to each other represent one observation well, while each dot represents a time.

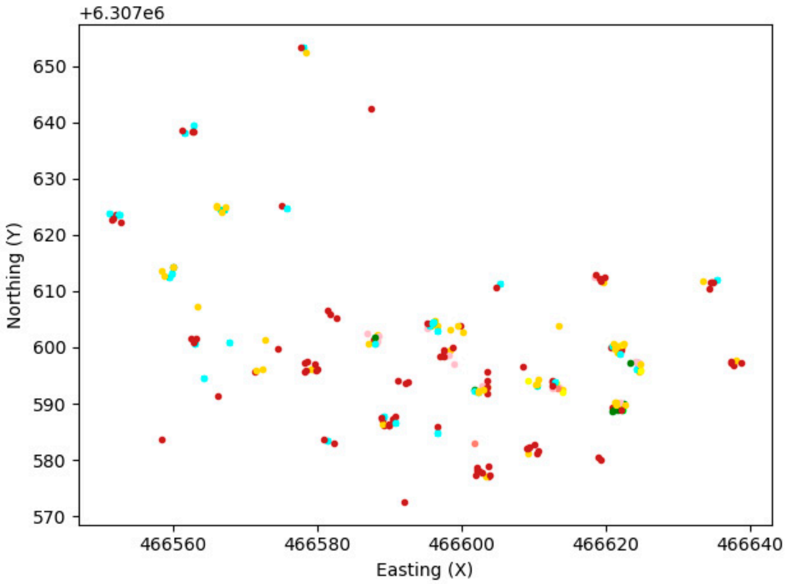


Fig. 17. K- means clustering output of all observation wells and all chemical parameters for 10 clusters.

Points with several dots clustered together (in different colors) indicate an observation well that was sampled multiple times. The figure suggests a large variability in the chemical's concentration over time at those locations because of different colors. This makes it hard to predict them. This variability may occur when the contamination changes phase recurrently (e.g., NAPL to dissolved, dissolved to absorbed, and absorbed to reduced/oxidized, etc.) even over very short time periods like our case study. Thus, various chemical and probably biological reactions and processes are likely to be active in many of the wells. This makes it especially difficult to predict their transport dynamics and fate.

5.3.2. Genetic algorithm versus INIDE-T

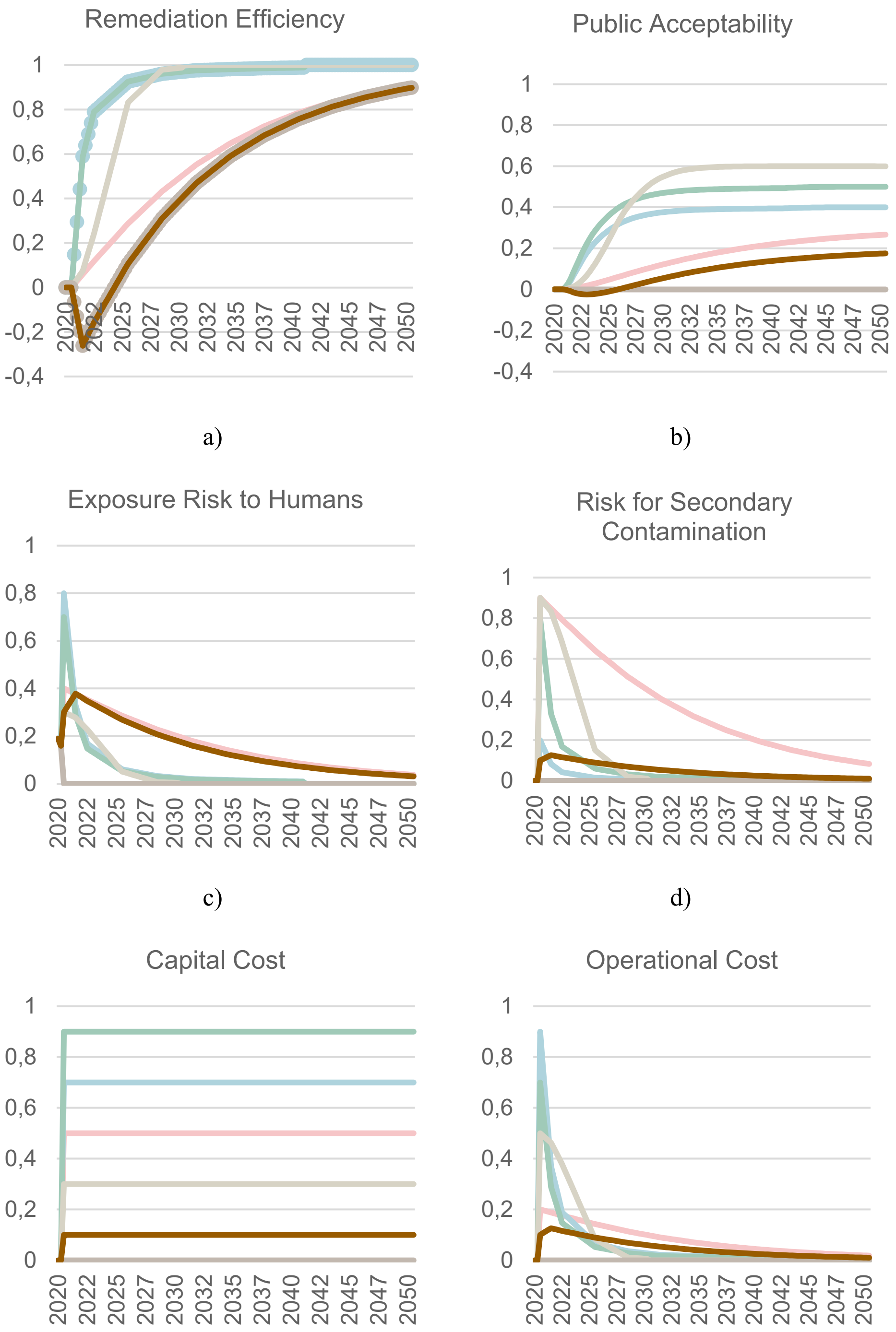
The large variability in the chemical's concentration over time may suggest that even advanced predictive algorithms may fail to correctly predict changes in such a complex system. We tested this hypothesis, applying a complex genetic algorithm for predicting the contamination fate. The results showed much lower confidence than the corresponding ones using the simple semi-analytic model implemented by INSIDE-T. Coefficient of determination (R^2) between measured and modeled concentrations was always below 0.4 in the genetic algorithm-based models, while it was 0.7 for INSIDE-T. This reaffirms that selection of a simple but efficient solute transport model like INSIDE-T is appropriate for such applications.

5.4. Dynamic modelling of sustainability

This thesis introduces a new approach for dynamic SA of contaminated site remediation options, building on previous advances, INSIDE and INSIDE-T, integrating them through system thinking principles. The new tool for dynamic sustainability assessment is called DynSus, for easy reference. One obvious benefit that addressing such dynamics may provide is helping understand the system response to different scenarios in the life cycle perspective.

In DynSus, system dynamics (SD) simulations are applied to explore the interrelationships among sustainability indicators simultaneously. SD is chosen as an integrative modelling method due to its specific ability to systematically describe the relationship between system structure and behavior (Forrester and Senge, 1980; Lemaire et al., 2021). Integrating contaminant transport modeling (INSIDE-T) with sustainability assessment (INSIDE), SD allows assessing the impact that temporal dynamics may have on acceptability of a remediation action in the life span of the project.

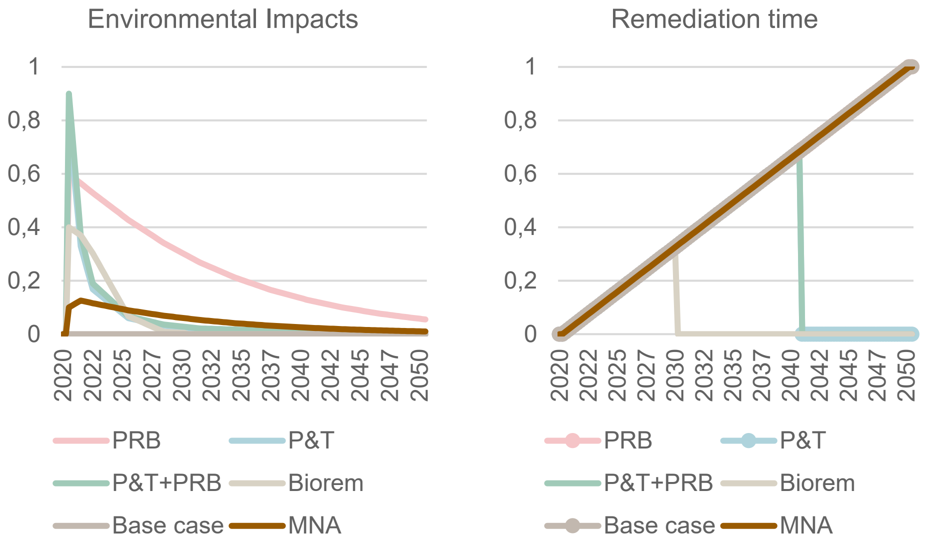
Figure 18a-h shows the simulation results (but only for 2020-2050) for all remediation scenarios considered, and for each criterion, and Fig. 19 displays the normalized sustainability for each scenario.


Remediation Efficiency
1
0,8
0,6
0,4
0,2
0
-0,2
-0,4
2020
2022
2025
2027
2030
2032
2035
2037
2040
2042
2045
2047
2050
Public Acceptability
1
0,8
0,6
0,4
0,2
0
-0,2
-0,4
2020
2022
2025
2027
2030
2032
2035
2037
2040
2042
2045
2047
2050
Exposure Risk to Humans
1
0,8
0,6
0,4
0,2
0
2020
2022
2025
2027
2030
2032
2035
2037
2040
2042
2045
2047
2050
Risk for Secondary Contamination
1
0,8
0,6
0,4
0,2
0
2020
2022
2025
2027
2030
2032
2035
2037
2040
2042
2045
2047
2050
Capital Cost
1
0,8
0,6
0,4
0,2
0
2020
2022
2025
2027
2030
2032
2035
2037
2040
2042
2045
2047
2050
Operational Cost
1
0,8
0,6
0,4
0,2
0
2020
2022
2025
2027
2030
2032
2035
2037
2040
2042
2045
2047
2050

a) b)

c) d)

e) f)



g) h)

Fig. 18. Changes in each criterion for the 6 different scenarios.

Remediation efficiency was set to 0 for the time before 2020, as there was no remediation option in place, and 1 for the time the remediation target concentration (in our case, 100 µg/L) is reached. For this reason, and considering that the PCP concentration can still increase for some time (years) after 2020 when no option is chosen (Naseri-Rad et al., 2021), the efficiency may be negative as seen in Fig. 5a for MNA (green line). *Public acceptability* is defined similarly to the efficiency except it can take site managers some time to ensure the concentration change is stable and to act accordingly. This lag, specified as perception time, was set to 2 years, and by that the Fig. 18b is attained.

Interactions across the variables *exposure risk to human*, *risk for secondary contamination*, *operational cost*, and *environmental impacts* are taken into consideration through the scenario coefficients, whose values are determined by expert judgment, and relate these criteria only to contaminant concentrations. These four parameters are considered as the concentration at any time divided by the initial concentration to result in normalized values for all. The only difference is *exposure risk to human*, and *risk for secondary contamination* may be unlikely when the concentration is very low. Thus, these criteria are simply set to zero for concentrations below 100 µg/L (remediation target). There is a risk for rebound (Fetter et al., 2018) and remediation action should last long enough after reaching remediation target to minimize that, while keeping the overall cost of the project reasonable. In this thesis, a concentration of 20 µg/L, which is one fifth of the remediation target, is considered as a suitable representation for this. Thus, the model is set to run if the remaining concentration at the recipient is not lower than 20 µg/L. Thus, remediation time continues to increase linearly, until remediating action is stopped, and capital cost is constant after it is put in the starting time of the action.

Finally, Fig. 19 depicts sustainability over time from the initial point when pollution occurs. As the figure shows, bioremediation may be the only remediation alternative that compensates the overall sustainability loss of the project in its life cycle (the sustainability plot goes back to 1); although this was not the most sustainable choice in the beginning (having nearly the steepest slope before 2030). On the contrary, more "gentle" measures like taking no action and MNA reached the least overall sustainability although they initially seemed to be the most sustainable options (see their mild slope before 2030). Remediation efficiency, however, plays an important role in this, and in case fewer intensive measures like natural attenuation could reduce contaminant level to the remediation target, the plot might be different for these "gentle" measures. Measures requiring more actions were less sustainable at the early stage (except for the PRB), while compensating their overall sustainability impacts at the end.

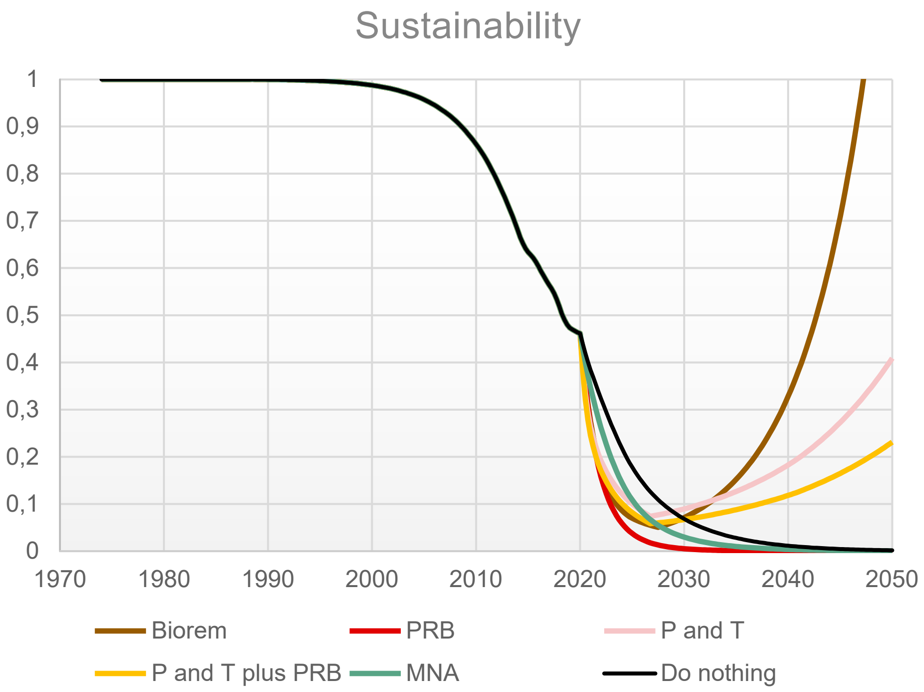


Fig. 19. Sustainability of each scenario in time from 1974 to 2050.

The unique capability of the model is that it can simulate the dynamic behavior for the governing parameters, which may be updated repeatedly based on available observed concentration data and/or any pilot measures. In the same way, perceived scores for different criteria may become altered through the life cycle of a remediation project, affecting other criteria, as captured by the feedback structure of the DST. For example, should bioremediation be selected for this case study and field conditions show that the environmental impacts of the measure are not as small as expected, managers may increase this (SC 5 in Fig. 5) and thus, change the whole system accordingly as needed.

Decision making under uncertainty

High uncertainty associated with contaminant mobility is intrinsic to contaminated sites modelling and SA studies. It is important to note that SD models often aim at enhancing the understanding of complex systems and sheds light on system behaviour in time (Srijariya et al., 2008) and not necessarily predictions (Sterman, 2000). Accounting for uncertainty of the decontamination process helps elucidate involved changes for all scenarios.

There are two main sources of uncertainty in the INSIDE-T. One type of uncertainty stems from the site-specific transport parameters, where inverse modelling is used prior to predictive modelling to ensure reliable estimations are produced. Moreover, three quartiles of values of all these parameters are applied in INSIDE-T for still showing the range of solutions that such uncertainty in transport parameters might generate. The other source of uncertainty is the assumed decontamination rates for the different remediation options.

Nevertheless, to further demonstrate DynSus capabilities regarding accounting for uncertainty, we introduced a perturbation of ±10% on assumed decontamination rates in all scenarios. Figure 20 shows the resulting change in the final sustainability scores for all remedy scenarios considering three quartiles of transport parameters and ±10% variability in assumed decontamination rates in all scenarios.

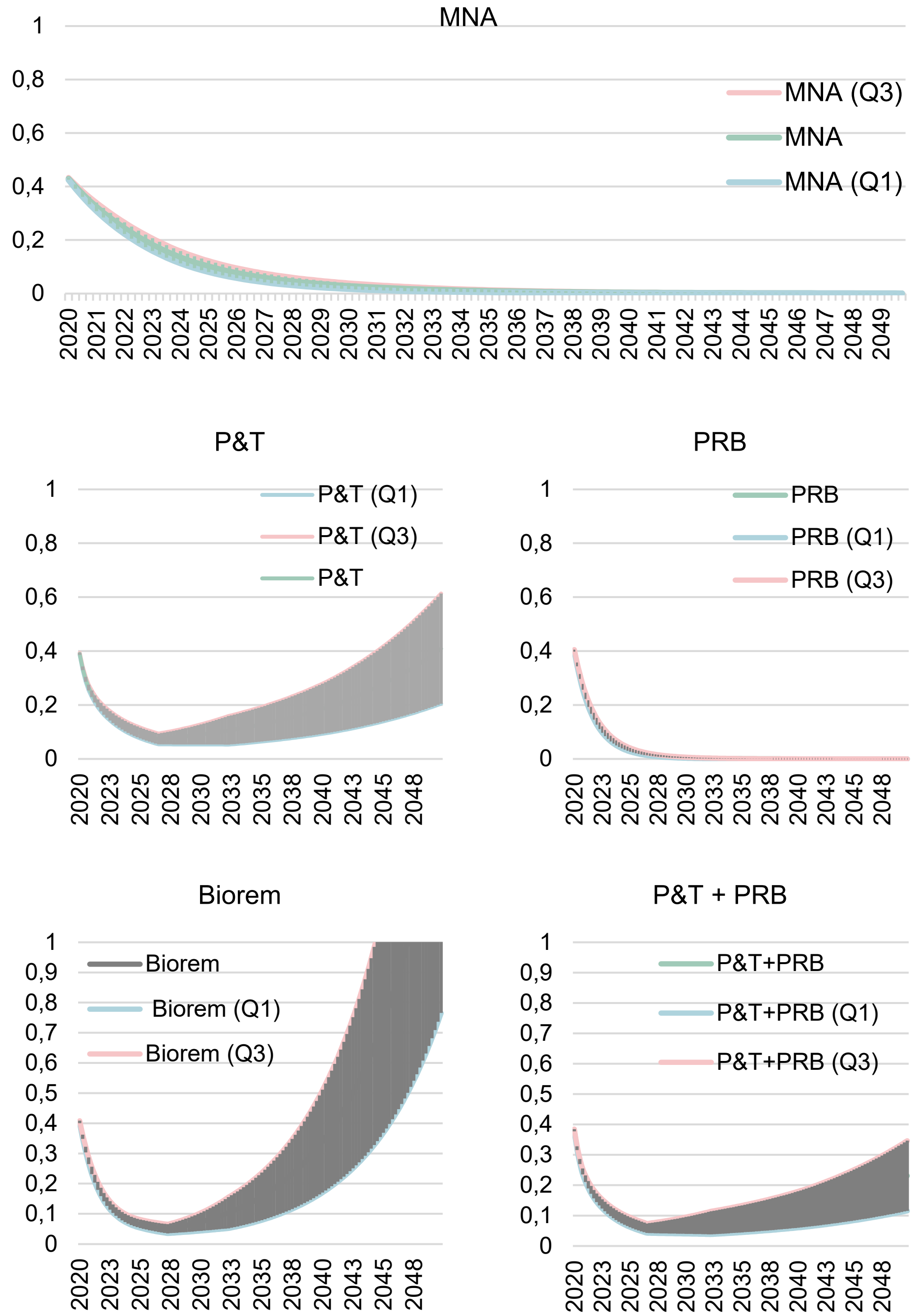


Fig. 20. Temporal uncertainty progression for the final sustainability scores for different remediation options resulting from a 10% perturbation in the transport parameters for INSIDE-T. Orange and blue lines represent modeling results through applying 1st and 3rd quartiles of transport parameters values, respectively.

Illustrated in Fig. 20, the results suggest that there may be less room for improvement in the MNA and PRB scenarios, compared to the other alternatives as their line spans are narrower. These results may help and encourage managers to improve other aspects of the system for more sustainable actions. Figure 20 does not indicate significant uncertainty in the starting years of all the remedy actions and except for scenarios that are not likely to reach the remediation target in 30 years, most of the uncertainty is shown to be during later years.

Finally, the life cycle perspective of sustainability dynamics for the case study suggests that bioremediation may be the only option that can compensate the overall social, environmental, and economic imposed burdens in the time span of interest (30 years). It should, however, be noted that models of real-world problems are, just simple representations of the remedy measures, and further studies need to be conducted. After bioremediation, P&T may provide sustainable outcomes, especially for the case where its sustainability could be improved across the different indicators. The combination of P&T and PRB and the PRB alone did not show promising results, although the former showed good contamination removal capabilities, especially in the beginning.

6. Conclusions

A new methodological approach for sustainability assessment with the aim of decision making for remediation actions at contaminated sites is proposed herein. This approach consists of a sustainability assessment tool and a contaminant transport model, that are consistent and integrated through system thinking principals.

The initiated SA tool, INSIDE, can be used as a guide for planning managerial actions in remediation and to prioritize remediation techniques. INSIDE shows a realistic non-hierarchical interaction structure of the remediation system and sheds light on the structures behind the considered weights for involved criteria. By that the complexity of the system is recognized. This enables to predict the consequences of the decisions and policies for different aspects more clearly. INSIDE showed that although time and cost are commonly assumed to be the main criteria in field applications, it turns out that these are not the most influential ones. Health and environmental concerns were instead evaluated as more influential. This suggests that human and ecological risks drive motivation to remediate, which in turn determines the resources needed for remediation.

The contaminant transport model INSIDE-T was developed for inclusion within an existing DST platform (INSIDE) dedicated to supporting decision-makers who must choose from various alternatives for sustainable site remediation. INSIDE-T can provide decision-makers with more reliable hydrogeological insights at the screening and preliminary management stage, and thereby enhance the overall sustainability scoring of potential remediation options. Simulation outcomes of INSIDE-T are contaminant concentration at the recipient for each scenario, and the concentration change pattern at any selected source-to-recipient location. Site managers can develop and simulate different remediation scenarios, regardless of their level of expertise, and visualize how a particular option may affect the desired outcome, i.e., concentration at the recipient. Incorporation of transport modeling can, thus, lead to a more reliable scoring of different options, while enabling a more transparent decision-making process. Another merit of this kind of simple solution is its adaptability with a limited number of observations, which is evaluated especially in Paper III. Detailed and costly site investigations are not possible for all contaminated sites. Using INSIDE-T with small data needs makes regional and national remediation plans applicable for a broad spectrum of contaminated sites.

More sophisticated modelling tools can then be applied upon need to answer specific questions concerning sire-specific conditions.

DynSus fully integrated an efficient contaminant fate and transport model (INSIDE-T) with an SA tool for site remediation practice (INSIDE) via a system dynamics framework. This integration can help site managers to recognize the dynamics related to the sustainability of each remediation scenario over the entire life cycle of the decontamination process. Importantly, it can be used for describing and communicating the real-world complexity, heterogeneity, and variability of contaminants behavior in the subsurface, and subsequently, remedial actions for dealing with them. The contaminant's removal efficiency was found to be a key driving factor in the dynamic sustainability assessment of remediation scenarios. This indicator was thus used as the bridge to integrate INSIDE-T with INSIDE. However, these efficiencies are subject to change due to complex and heterogenic conditions of the subsurface environment. This necessitates a frequent updating of the performance of the model. Notably, this method provides a transparent framework that lets site managers update scores of each indicator as needed, after each field campaign, which will then automatically impact the other criteria according to the defined interrelations (feedback structure of the SD model). This essentially helps to understand the system, test different scenarios and ways to improve them over their life cycle, while considering different timeframes and remediation targets in a dynamic manner.

7. Delimitations and ways forward

In INSIDE, although relying on experts' opinions has the benefit of using their knowledge and expertise in a simple way, subjectivity in opinions is also probable. For this reason, attention is paid to include different respondent groups from different sectors and from different countries. Still, the mentioned uncertainty is inherent in the method and must be further studied in future research, otherwise discussed with the stakeholders when it is put to application.

Surveys of professionals are basically harder to arrange and control than public surveys. This is because professional participants are not often willing to spend time on seemingly unproductive work without payment. This fact implies that the questions must be as few and easy-to-answer as possible. Consequently, this delimits the survey result information content. Overall, the design and execution of interviews become very important for interpretation of results. The presented methodology for handling human judgement can, however, be a starting point towards more realistic decision-support systems that recognize indicators interactions and real-world decision-making complexities.

INSIDE-T, although simplicity is considered as a merit and aimed for, can cause problems if the site complexity (hydrogeochemical conditions) is not properly represented by the collected data. Although, the modeling approach was also applied to a data scarce site, like all modelling tools, site investigations must be performed to give basic information on transport properties. In addition, although careful attention was paid to make efficiency assumptions when visualizing scenarios, these may not reflect the true performance efficiency in the field, as treatment performance efficiencies are expected to be site-specific. Experts with experience in similar sites are relied on for making such assumptions in INSIDE-T. This must be considered and communicated to decision makers that would use such tool.

In DynSus, although an SA needs some degree of subjectivity to incorporate all aspects and DynSus is not an exception in this matter, this subjectivity must be treated with consideration. Only experienced site managers may be asked for scoring the remediation alternatives. Also, pilot remediation actions may deliver different results in different parts of the site or at different times. Using these inputs for running DynSus may result in different outcomes. It must be noted that the inputs should be representative of the entire site over the time span of interest. Finally, site-specific conditions may sometimes dictate the remediation measure chosen and there may not be many options to consider. The assumption is that all alternatives presented here are feasible and only differ in their efficiency in time and space.

The present methodology provides a holistic view for incorporating more robust data in view of different sustainability aspects (environmental, social, and economic) and methods to quantify them. Quantifying these aspects may lead to more reliable results, although perhaps labor intensive. However, site remediation is a site-specific problem and quantifying sustainability of different actions may necessitate different modules to be added. Applying DynSus on more sites may help in this regard, too.

Ideally, having a module for investigating technical aspect of the problem in terms of contaminant transport (INDIE-T) could be repeated for environmental, social, and economic aspects separately. This might minimize the need for expert opinions and maximize reliability of the whole methodology. Life cycle assessment (LCA), and cost benefit analysis may be suggested for quantifying environmental and economic aspects, respectively. However, such advancements might increase the cost of setting such assessment and may be more applicable for bigger projects or even regional remediation plans.

To further reduce subjectivity of assumptions at different stages for which expert judgement was used, fuzzy logic could be of help. Moreover, data-driven methods could provide improved decision making under uncertainty. These are, however, yet to be discovered and implemented in the field. Although, not applicable for many sites, data mining methods could help with understanding site dynamics in the cases a wealth of hydrogeochemical data is investigated.

Finally, the current thesis is just a beginning of innovative dynamic sustainability assessment. The presented methodology for integrating technical aspects of the problem with its SA concerns could be applied to many more fields. This could be any type of problem where the sustainability of a technology should be selected and assessed in comparison to other alternatives.

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About the Author

MEHRAN NASERI-RAD is a great lover of sustainability and the environment, who cares a lot about the planet that is to be left for the next generations! He obtained a bachelor's degree in Civil Engineering in 2013 and a master's degree in Environmental Engineering in 2015. Although trained as an engineer, a great passion for managerial aspects of the engineering projects could not let him go for a pure engineering career. This passion meant much more to him when he was introduced to decision support systems and sustainability assessment methods in his Ph.D. research. So, instead of picking either engineering or management, he chose to stay in both and even make a bridge between the two! He tries to make it possible by using his engineering knowledge in the environmental management of projects and technologies in the best form that he could possibly find, sustainability assessment!

The picture on the cover of this thesis is some of my handwritten notes when we had a supervision meeting in 2019 and I was storm braining about the fantastic models(!) that were then yet to come. These thoughts came to existence in later years as INSIDE, INSIDE-T, and DynSus! It was originally Magnus Persson's idea who suggested such a note could be a cover photo for my thesis three years later!

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