Science of the Total Environment 832 (2022) 154992

Contents lists available at ScienceDirect

Science of the Total Environment

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

DynSus: Dynamic sustainability assessment in groundwater remediation practice

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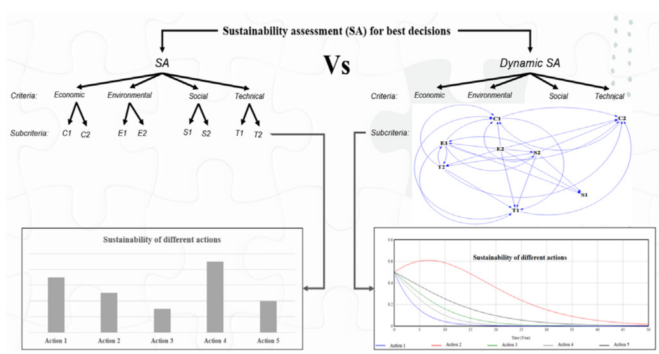
HIGHLIGHTS

- Hydrogeochemical and managerial uncertainties suggest a dynamic framework for promoting sustainable clean-up actions.
- DynSus integrates a predeveloped contaminant fate and transport model with a sustainability assessment tool.
- Passive practices, e.g., natural attenuation, failed to compete with active practices, over the entire life cycle of the project.
- Statistical tools are used to assess hydrogeochemical data and suitability of the applied contaminant transport model.
- DynSus outcomes enables site managers to evaluate scenarios more quickly and effectively for life cycle sustainability.

GRAPHICAL ABSTRACT



ARTICLE INFO

Editor: Jurgen Mahlknecht

Keywords:
Sustainability assessment
Sustainable remediation
System dynamics
Contaminated sites
Groundwater

ABSTRACT

Decision-making processes for clean-up of contaminated sites are often highly complex and inherently uncertain. It depends not only on hydrological and biogeochemical site variability, but also on the associated health, environmental, economic, and social impacts of taking, or not taking, action. These variabilities suggest that a dynamic framework is required for promoting sustainable remediation. For this, the decision support system DynSus is presented here for integrating a predeveloped contaminant fate and transport model with a sustainability assessment tool. Implemented within a system dynamics framework, the new tool uses model simulations to provide remediation scenario analysis and handling of uncertainty in various data. DynSus was applied to a site in south Sweden, contaminated with pentachlorophenol (PCP). Simulation scenarios were developed to enable a comparison between alternative remediation strategies and combinations of these. Such comparisons are provided for selected sustainability indicators and remediation performance (in terms of concentration at the recipient). This leads to identifying the most critical variables to ensure that sustainable solutions are chosen. Simulation results indicated that although passive practices, e.g., monitored natural attenuation, were more sustainable at first (5–7 years after beginning remediation measures), they failed to compete with more active practices, e.g., bioremediation, over the entire life cycle of the project (from the beginning of remedial action to achieving the target concentration at the recipient). In addition, statistical tools

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http://dx.doi.org/10.1016/j.scitotenv.2022.154992
Received 10 January 2022; Received in revised form 18 March 2022; Accepted 29 March 2022
Available online 2 April 2022

(clustering and genetic algorithms) were used to further assess the available hydrogeochemical data. Taken together, the results reaffirmed the suitability of the simple analytical framework that was implemented in the contaminant transport model. DynSus outcomes could therefore enable site managers to evaluate different scenarios more quickly and effectively for life cycle sustainability in such a complex and multidimensional problem.

1. Introduction

Soil, sediment, and groundwater pollution involving various types of anthropogenic contaminants represents an increasing risk to human health and the natural environment, as well as restricting efforts to redevelop brownfield sites. Since the aim is environmental improvement, it may be assumed that remediation is a "sustainable" action. However, like other kinds of land management developments, remediation is associated with extensive economic (Barrieu et al., 2017; Söderqvist et al., 2015), social (Harclerode et al., 2015; Norrman et al., 2020), and environmental (Fitzpatrick et al., 2018; Lemming et al., 2010) impacts. Sometimes, the negative impacts may outweigh the benefits (Anderson et al., 2018; Bardos et al., 2016; Cundy et al., 2013; Favara et al., 2019; Surf-UK, 2010).

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) although green remediation is more concerned with managing risks to human health and the environment while minimizing associated environmental impacts. Sustainable remediation, on the other hand, takes economic and social aspects into account as well. This involves not only maximizing the net environmental benefit but also reducing net life cycle project costs and maximizing gains in the wider economy while social impacts to workers and local communities are addressed (Hou, 2020). Thus, the goal of conducting a sustainability assessment (SA) within a site remediation context is to maximize its benefits while minimizing its negative unwanted impacts. The path toward sustainability, however, consists of numerous underlying decisions made by individuals, groups, and organizations (Hou, 2020), which are not always transparent nor easy to comprehend in terms of governing criteria (Burlakovs and Vircavs, 2012). SA is a crucial tool to support decision-making for such complex, multidimensional problems.

Life-cycle assessment (LCA), standardized by the ISO 14040 series (ISO 14040, 2006), may be considered as one of the most comprehensive SA tools (Hou, 2020); though its focus is mainly on quantifying environmental impacts (Hou and Li, 2017) and considers other pillars of sustainability only after coupling with other methods (Visentin et al., 2019). It is often data and time intensive and not readily doable for every site (Søndergaard and Owsianiak, 2018). SA tools based on multicriteria decision analysis (MCDA) (e.g., An et al., 2017, 2016; Rosén et al., 2015), on the other hand, reduce the cost and complexity of decision-making (Bardos et al., 2016) but depend on robust unbiased input (Tamm et al., 2008). This makes them less reliable for site managers who need conclusive decision support as early as possible, i.e., when access to robust data is typically less available.

It should be noted that, not including a reliable contaminant fate and transport model within the scope of SA may result in their failure to recognize the main drivers of the problem dynamics. And as a result, they often fail to highlight key system feedbacks, arising from the nonlinear problem structures known to exist in contaminated land management (McKnight and Finkel, 2013; Naseri-Rad et al., 2021). It is well known that the hydrological and biogeochemical variation at the site might have a great impact on the choice of remedial measure and its efficiency over time. The impact of such variations may be summarized using contaminant fate and transport models that exist for this purpose. However, these tools can further complicate the decision process, as they may be fragmented into subdisciplines that introduce additional biases thus preventing the holistic evaluation of a site remediation (Lemaire et al., 2021). Integration of these contaminant transport models with SA tools has generally not yet been practiced. Therefore, there is an urgent need for new modeling approaches that can quantitatively assess the sustainability of complex and multidimensional decision-making problems in a more integrated way (Onat et al., 2016), and remediation scenarios are no exceptions.

Consequently, this paper introduces a new approach for enabling the dynamic SA of contaminated site remediation options, building on previous advances. We apply an MCDA-based SA tool, INSIDE (Naseri-Rad et al., 2020), and a suitable contaminant transport model, INSIDE-T (Naseri-Rad et al., 2021), for this purpose and integrate them here through system thinking principles. We call this new method DynSus, for easy reference. INSIDE is a SA tool that helps explore interactions among sustainability indicators, replacing common assumptions of hierarchical structure for decision analysis in remediation projects (e.g., analytic hierarchy process: An et al., 2016; Li et al., 2018). For example, in a hierarchical structure, a criterion like remediation time can be assumed to be related to environmental, social, economic, and technical categories. It could be rationally categorized into each of these categories, as well as influence all the others. The same applies to other sustainability indicators. Such inconsistency between models and real-world conditions may result in inapplicability of such models and misleading results.

One obvious benefit that addressing such key system dynamics may provide is helping site managers to better understand the system response to different scenarios in time. 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 a reasonable assumption for all contaminated land cases. Of course, at certain sites, the former may fail or take a longer time than deemed acceptable to reach the desired outcome, which no longer makes it a favorable option, and/or the acceptability of a specific technology may change.

INSIDE further contains realistic non-hierarchical interrelationships between decision criteria in groundwater remediation. These criteria, also known as sustainability indicators, 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. INSIDE-T is a semi-analytic contaminant transport model that can be integrated with SA tools (like INSIDE) and is used here for quantitatively estimating contaminant concentrations at a defined recipient (e.g., a lake down-gradient or groundwater at some distance from the source zone).

In DynSus, we apply system dynamics (SD) simulations as an integrative modeling method due to its ability to systematically describe the relationship between system structure and behavior (e.g., Forrester and Senge, 1980; Lemaire et al., 2021) based on the concept of information feedback and control (Khan et al., 2009; Simonovic, 2000). Integrating contaminant transport modeling (INSIDE-T) with sustainability assessment (INSIDE), SD highlights the impact of real-world dynamics on overall sustainability of a remediation action.

Use of SD, as a modeling technique, is emerging in the field of water resources management (Carnohan et al., 2020; Simonovic, 2000), and hydrogeology (Khan et al., 2009) mainly due to recognition of its immense potential in linking all aspects of the decision-making process (McKnight and Finkel, 2013) using an interlinked system of stocks and flows (McKnight et al., 2010). SD is a technique that simulates system behavior by piecing all complex sub-systems together to enable a transparent and flexible process (Beall et al., 2011; Winz et al., 2009). This inherent capability is of paramount importance in SA practice (Honti et al., 2019) and makes SD a powerful (Bossel, 2007; Musango et al., 2012) and popular (Nabavi et al., 2017) method to assess the sustainability of applied technologies. In other words, SD is a strategy for information processing, including information feedback (Ford, 2010) with the focus on piecing together of (relevant) subsystems 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 is capable of permitting both deterministic and probabilistic investigations (Lemaire et al., 2021) of the dynamic behavior of a system, where causes and effects can change based on time-dependent boundaries of the system. Thus, SD introduces a flexibility lacking in other methods, including increased speed of model development and improvement, ability to simulate interactions between model components, and better transparency resulting in improved confidence for all the stakeholders involved.

To our knowledge, SD has not yet been exploited in the sustainable remediation industry. Even in the broader field of contaminated sites studies, there are only a few applications. McKnight et al. (2010) evaluated the impacts of point sources in groundwater on human health and surface water ecosystems using an SD-based DSS. BenDor et al. (2011) used SD for assessing the redevelopment policy of brownfields from an urban planning point of view. McKnight and Finkel (2013) developed an SD model to assess human health risks at contaminated sites, which was based on contamination spread in time and space. And Tseng et al. (2018) used SD to estimate health savings benefits associated with remedial actions. Considering this, the main objective of this study is to integrate contaminant transport modeling, as a driver in the remediation system, with SA, for a more reliable holistic view of the remediation practice. Such a holistic view can be used to guide decision-makers through the life cycle of the remediation project. Other objectives of this paper are to:

- develop a causal loop diagram (CLD) together with a stock-and-flow diagram for the remediation process by means of quantified interrelationships between sustainability indicators,
- incorporate contaminant transport modeling (INSIDE-T), within the proposed system dynamics framework, to provide general estimates of contaminant concentrations at the water recipient and thereby enable a more quantitative assessment of sustainability indicators,
- apply system dynamics to model the entire system and assess the overall sustainability of selected remedial measures in its life cycle,
- conduct uncertainty analyses for better communication of results, and
- test the methodology on a case study to demonstrate its validity for improving the SA of remediation options at contaminated sites.

In view of the above, the hypothesis of the present paper is that a holistic dynamic approach for site remediation can improve the overall resilience of pollution management.

2. Methods and materials

2.1. Improved understanding of site dynamics

A K-means clustering method was 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 necessary due to the numerous often-complex processes found at contaminated sites. This method enables an improved understanding (Balbarini et al., 2020) of the concentration dynamics (pattern over time) and allows their variability to be determined.

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 (Likas et al., 2003). A list of the hydrogeochemical variables assessed in this study is provided in Appendix A. The K-means algorithm grouped the data into 10 potential clusters in this study.

Secondly, we used *Eureqa*® Software to test its ability to predict concentrations spatially and temporally and compared with results from INSIDE-T. Eureqa® explores the space of possible solutions using a genetic-algorithm-based technique, based on a training dataset (comprised of 70% of the data). Once a solution is identified, it is validated using independent data (remaining 30% of the data) in terms of prediction performance. Genetic algorithms are widely used in optimization problems because of advantages in terms of easy convergence and high accuracy (Gen and Cheng, 1999). We apply *Eureqa*® here to investigate the relationships between observed parameters and contaminant concentrations in groundwater at certain times and locations.

2.2. INSIDE framework and contamination transport by INSIDE-T

In INSIDE, each criterion can freely influence and/or be influenced by all other criteria, where the sustainability criteria and their calculated weights in decision analysis are as follows: *Capital costs* (*12.8%*), *Operational costs* (*12.7%*), *Remediation time* (*12.3%*), *Remediation efficiency* (*12.4%*), *Environmental impacts* (*12.7%*), *Risk for secondary contamination* (*12.5%*), *Public acceptability* (*11.9%*), and *Exposure risk to humans* (*12.6%*). These criteria and their weights, which were calculated using criteria interrelationships, are results from a previous published study (INSIDE) by Naseri-Rad et al. (2020). The values of weights are actually not significantly different from each other. These are similar to values considered in other studies (An et al., 2017; Li et al., 2018) where social, environmental, and economic criteria would get equal weights and sub-criteria in each of these would gain almost similar wights compared to each other, as well.

Besides using the genetic-algorithm for quantitatively assessing contaminant concentrations at the recipient, we employ INSIDE-T in this study. INSIDE-T is a two-dimensional transport model based on the advective dispersive equation for solute transport according to (Bear, 1988; Ogata, 1970; Ogata and Banks, 1961):

$$c(x,y,t) = \frac{C_0\left(\frac{Q}{b}\right)}{4\pi(D_L D_T)^{1/2}}\, exp\left(\frac{v_x x}{2D_L}\right)[W(0,B) - W(t_D,B)] \tag{1}$$

and

$$\mathrm{t_D} = \frac{\mathrm{v_x}^2\mathrm{t}}{4\mathrm{D_L}} \text{ and } \mathrm{B}^2 = \frac{\mathrm{v_x}^2\mathrm{x}^2}{4\ \mathrm{D_L}^2} + \frac{\mathrm{v_x}^2\mathrm{y}^2}{4\ \mathrm{D_L D_T}}$$

where C (M/L^3) is solute concentration, Q (L^3/T) is the rate of injected contaminant, b (L) is the thickness of the aquifer over which the contaminant is injected, D_L (L^2/T) and D_T (L^2/T) are longitudinal and transversal hydrodynamic dispersion, respectively, and v_x (L/T) is the average linear velocity. $W(t_D, B)$, and $W[u, r/b]$ are known as leaky well function and can be found in Hantush (1956).

This equation is valid for homogeneous and isotropic media with Darcy's law. Thus, INSIDE-T provides only a simple analytic and semi-analytic framework for dissolved contaminant transport simulation for targeted remedial scenarios for rapid estimates in SA practice. However, INSIDE-T is based on inverse modeling to estimate site-specific transport parameters to maximize adaptability with field conditions. Next, these parameters are used for prediction of contaminant spread in time and space. INSIDE-T approach has been used for modeling the transport of total petroleum hydrocarbons (TPH) in data-scarce areas (Radelyuk et al., 2021). However, it is still more suitable for primary and screening level studies and may therefore not be as versatile a tool for all site conditions.

2.3. Building the SD model

We use Vensim® software for the SD simulations in this paper. Feedback is a crucial concept in the application of SD simulation tools, as this is the primary mechanism often underlying the nonlinear behavior typically found governing (natural) systems. To better explore and communicate the inherent feedback structure of a particular system, 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 behavior (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 behavior/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 behavior of a loop, one must count the negative signs in the loop. Whether this is odd or even determines whether the loop has balancing or reinforcing behavior, respectively.

CLDs can thus be used to help identify the critical system variables and their feedback loops that may be governing the dynamic behavior in a system under investigation (Ford, 2010), as well as ensure that policy or management decisions taken will have the desired effect (e.g., reduction or removal of unwanted reinforcing behavior). 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. 1.

It should be noted that in complex systems where remediation practices are needed, negative and positive signs may change over time. 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 data generation to enable this).

Another central concept in developing SD models are 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):

$$\mathrm{Stock}\ (t) = \int_{t_0}^{t} [\mathrm{Inflow}(t) - \mathrm{Outflow}(t)]dt + \mathrm{Stock}(t_0) \qquad (2)$$

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.

In our case, although the stock could be any of the recognized sustainability indicators, combinations thereof (i.e., multiple coupled stocks), or the contamination concentration itself, we focus entirely on the target parameter of the simulation – sustainability – and thus this is the only stock. Sustainability of any remediation action can then be measured as the change in ‘accumulation’ occurring in the stock. In this model, we use the inflows to and outflows from the stock to represent factors responsible for either increasing or decreasing the sustainability, respectively. These factors are comprised of the 8 sustainability indicators and their weights (see Section 2.2). A stock-and-flow diagram, highlighting the interactions and influential factors, is shown in Fig. 2.

The first step in the application of DynSus is to choose from the five available remediation options (e.g., technological solutions). In Fig. 2, bioremediation was chosen, and this is connected to the variable it influences, which is concentration at the recipient (C(R) in selected scenario). As explained further in Section 3, remediation technologies considered 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) was already estimated through INSIDE-T and is imported here for further analyses.

Although, different remediation scenarios take different time to reach the target concentration, all scenarios have been modelled for 30 years, representing the total (acceptable) project life cycle, starting from 2021 (as no remediation occurred prior at the site). 2021 to 2050 is a reasonable assumption for an acceptable life cycle as most remediation alternatives at the site are expected to be finished by then, and this time span is in line with the national plan for the decontamination of such sites (high risk and very high-risk sites) by 2050. Moreover, having all the scenarios on one timescale makes it easier to compare them. More specifically, having estimated the initial contamination of the groundwater occurring in 1974 (Nord, 2019), the full simulation period spans 76 years, and includes 46 years of ‘no action’ (1974–2020) and 30 years of (active or passive)

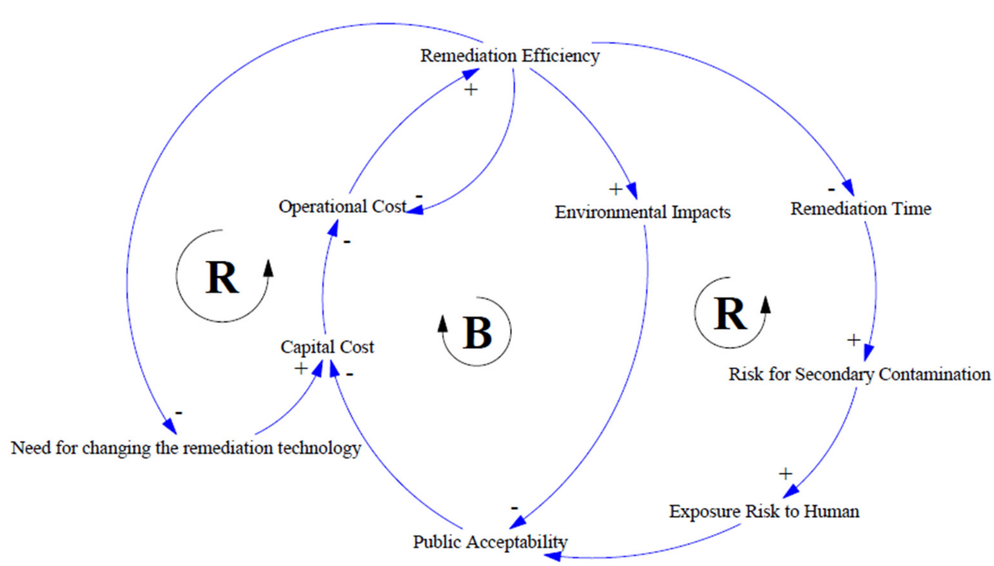


Fig. 1. Causal loop diagram of remediation practice, based on recognized sustainability indicators (Naseri-Rad et al., 2020). Letter R and B represent reinforcing and balancing behavior of the loops, respectively.

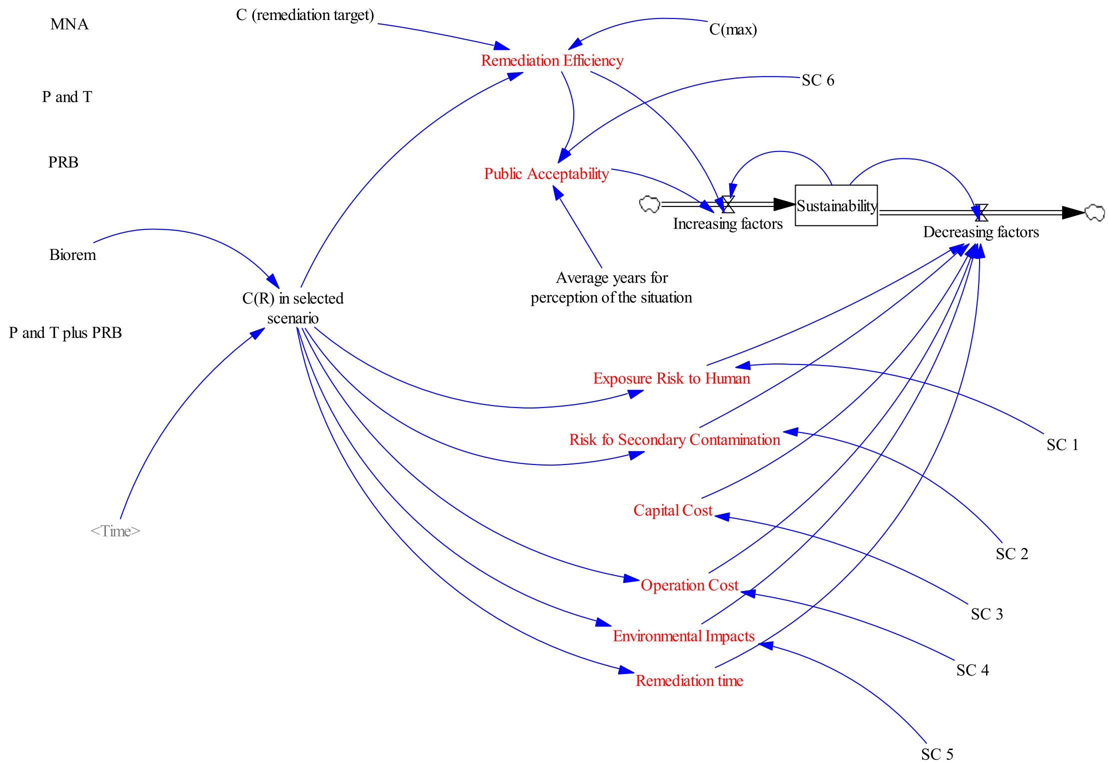


Fig. 2. Stock-and-flow diagram of the SD simulation model, DynSus, combining recognized sustainability criteria used within INSIDE (in red) with key contaminant concentration output from INSIDE-T (Naseri-Rad et al., 2020). SC1 to SC6 represent the scenario coefficients of the sustainability criteria that are different for each remediation scenario. This figure further shows the interlinkages, when bioremediation (Biorem) is chosen as the remedial strategy (from the five options listed on the left), and thus drives changes in the concentration at the receptor (C(R) in selected scenario).

remediation action (2021–2050). In the case where remediation targets are met, the remediation actions will be stopped with a short delay (to account for perception time) in the model.

C(*R*) *in the selected scenario* represents its "remediation efficiency" and 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) has been set to 1790 μg/l that was the concentration of PCP at the end of 2020 and before performing remedial actions. Recipient in this study is a nearby lake that the contamination plume is flowing to (described in Section 3), and its exact location is presumably the first place that groundwater contamination plume reaches the nearby lake. The remediation efficiency is set to 0 for the time before 2020, as there was no remediation in place, and to 1 when the remediation target concentration (in our case, 100 μg/l) is reached.

Remediation efficiency is the most important objective measure that affects all eight criteria and the choice of remediation technology. According to the CLD in Fig. 1, it affects all eight criteria and the choice of remediation technology, except the *capital cost*. The capital cost represents the total budget needed to get a remediation technology up and running and is mainly fixed. Notably, if the remediation efficiency is not satisfactory at some point, it may be necessary to change the remediation technology, which may directly alter the capital cost as demonstrated by the factor *Need for changing the remediation technology* in the CLD (see Fig. 1).

However, remediation efficiency is not the only variable that affects all criteria. There is an associated impact for each technology on every criterion. 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 the contamination is pumped up to the ground in this scenario). These impacts are considered here by coefficients SC1 to SC6 (*scenario coefficients*). The scenario coefficients have a similar function as the weighting factors used in standard MCDA models and may be assigned by a group of experts. They might differ in case-specific approaches (Appendix I). These coefficients should not be mixed up with the criteria weights. Criteria weights, calculated by INSIDE, are used here for the last stage of the sustainability assessment as multipliers of increasing and decreasing factors (shown in Fig. 2), while scenario coefficients are scores in different sustainability criteria that a certain remediation scenario may achieve. For this, we used a questionnaire and asked remediation experts to determine coefficients for each remediation technology as regards other alternatives (Naseri-Rad et al., 2021). The only criteria with no *scenario coefficient* assigned are *remediation efficiency* and *remediation time*. This is because these are estimated by the contaminant transport model INSIDE-T, 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., 2018; Li et al., 2018; Onwubuya et al., 2009; Rosén et al., 2015).

Moreover, it is a reasonable assumption 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 assign to each technology. Reversely, 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*)) – also called remediation efficiency.

However, there is one key difference between these two categories. It may take some time after contaminant concentrations reach a certain level before it may change *Public Acceptability*. This is accounted for in the factor *Average years for perception of the situation*. This is assumed to be two years; meaning that it may take about two years after contamination concentrations reach a certain limit that the public may recognize the change and react accordingly. For example, it will probably take some time after concentration levels reach an acceptable level for local land prices to change. 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 span that the contaminant concentration at the recipient has not reached the target remediation target. *Remediation Efficiency* and *Public Acceptability* are thus *Increasing factors* while the other criteria represent *Deceasing factors* in measuring the sustainability of a remediation practice (as shown in Fig. 2).

3. Case study

In the 2000s, high levels of contaminants were detected at a former sawmill plant in Hjortsberga, located in Alvesta Municipality, Kronoberg County, southern Sweden. The plant was in operation since the early 1940s to late 1970s (Elander and Eriksson, 2007) and has left a legacy of high concentrations of pentachlorophenol (PCP) and dioxins (Johansson, 2006) in the subsurface. Unlike PCP, which transported to the groundwater due to its chemical properties (e.g., high solubility, etc.), dioxins were mostly found in the unsaturated soil zone (SGU, 2017). In 2013, the Swedish Geological Survey (SGU), as the site manager, had the dioxins-contaminated soil excavated (Nord, 2019). This removed nearly all hazardous levels of dioxins from the soil, but threatening concentrations of PCP still exist in the groundwater (SGU, 2017).

A more detailed description of the site situation together with the observed data and assumptions on remedy scenarios' performances can be found in Johansson (2020) and Naseri-Rad et al. (2021), respectively. Also, summaries of investigated data, transport parameters ranges, and assigned scores to different remedy measured in selected sustainability indicators may be found in the Appendix. As shown in Fig. 3, PCP contamination in the groundwater is threatening the nearby Lake Sjöatorpasjön and site managers are considering these alternatives as remedy measures for the site: 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*). A short explanation of these methods is as follows:

- MNA – contaminants attenuate by sorption, volatilization, dilution, and dispersion coupled with biodegradation.
- P&T – pumping up contaminated groundwater to a nearby treatment plant that applies conventional wastewater treatment methods to remove contaminants.
- PRBs – installing permeable reactive barriers across the flow path to remove the contaminants from the groundwater.
- Bioremediation – stimulating existing bacteria in the environment, by injecting air or nutrients, to consume more contaminants (biostimulation), or introducing more archaea or bacteria culture to the environment to enhance contaminants biodegradation (bioaugmentation)
- P&T + PRB – Placing a PRB in front of the plume while performing P&T simultaneously at the source.

Heterogeneity of the aquifer can substantially affect P&T efficiency. Especially with a mix of fine and coarse materials at the site, many issues, e.g., back diffusion and tailing are likely (O'Connor et al., 2018). These issues are also relevant for PRBs. Reactivity loss of reactive materials, clogging, and plume bypass around, under, or over the barrier, and through seasonal fluctuations in groundwater flow are among the other main issues affecting PRB performance (FRTR, 2002).

Site managers have already performed an unsuccessful biostimulation pilot test at the site, concluding that, indigenous bacteria are not suitable enough for the purpose (Elander and Eriksson, 2007). Therefore, bioaugmentation (introducing an exogenous bacteria culture to the environment) is considered here. This is, however, not unlikely to perform below expectations due to the complex geology at the site.

The contaminant transport modeling performed by INSIDE-T calculates concentrations at the source and at the recipient while no remedy measure is in place. For all alternatives (all remedy scenarios except MNA), INSIDE-T assumes a decontamination rate based on literature review of similar sites and estimation by remediation experts. The potential decontamination rates are always subject to uncertainty and cannot be generalized for such a site-specific problem. However, relying on literature values for similar sites and experts knowledge, as suggested by Naseri-Rad et al. (2021) may be a reasonable assumption in this context.

Although chlorophenol usage has been banned in Sweden since 1978 (Swedish EPA, 2009), these contaminants are persistent in the environment and are still widely detected (Liu et al., 2019). According to the Stockholm convention, PCPs are recognized as persistent organic pollutants (POPs) in the environment (UNTC, 2001). Fortuitously, indigenous microbes can sometimes remove low levels of PCP (< 1000 μg/L) to approach the regulatory standard of 1 μg/L with the addition of oxygen, with or without nutrient amendment (Schmidt et al., 1999), with a typical PCP half-life ranging between 0.1 and 3 years (USEPA, 1991). It should be noted that PCP is a fungicide that inhibits the activity of microorganisms above certain concentrations. For example, PCP concentrations as low as 20,000 μg/L in water can inhibit microbial activity (Davis et al., 1994).

4. Results and discussion

4.1. Observation wells dynamics

To categorize different wells in different clusters based on their investigated hydrogeochemical data, we performed a K-means clustering with 10 clusters. All the data (in all times) is used for this purpose to see if chemicals

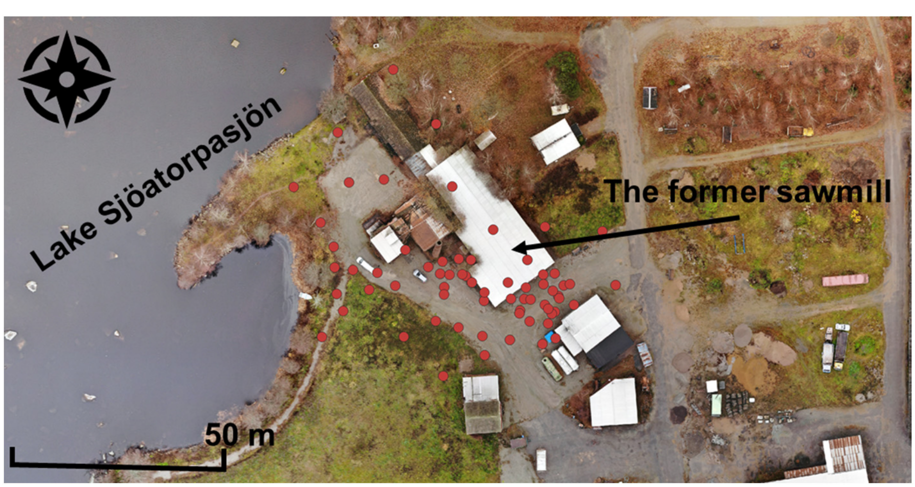


Fig. 3. Location of the former sawmill plant, and sampling wells (red dots) used as a case study.

contents are changing in similar way in specific wells. Noticeable change compared to the relative chemical levels may suggest complex hydrogeologic condition, as big changes in chemicals levels are normally not expected in short time periods. The results of the clustering by the k-means method for all observation wells and based on all chemical parameters (see Appendix A), are illustrated in Fig. 4. Note that a small noise of 1 m has been implemented to avoid direct overlapping of the color-assigned categorization for different sampling times. The dots that are significantly close to each other thus represent one data point (observation well in space), while the color represents the temporal category that the well falls into based on its overall chemicals content at the time of sampling.

The figure shows that many points have only had one observation in time and consequently have only one dot (representing an in-situ grab sample). Similarly, there are many points with several dots clustered together (in different colors) indicating an observation well that was sampled multiple times. The different colors at the location of a certain well suggest a large variability in the chemical's level over time which makes it hard to predict their variability. 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 and spatial distances. 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. This may suggest that even advanced predictive algorithms may fail to correctly predict changes in such a system.

We tested this hypothesis, applying the 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 (Appendix I). Coefficients of determination (R^2) between measured and modelled concentrations were always below 0.4 in the genetic algorithm-based models, while they were around 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.

4.2. Dynamic modeling of sustainability

Fig. 5a–h shows the simulation results (2020–2050) for all considered remediation scenarios, and for each criterion, while Fig. 6 displays the normalized sustainability for each scenario.

As shown by the CLD in Fig. 1, the *remediation efficiency* of a particular method is a key parameter in the system, affecting all other criteria. Because of this, all the other criteria are mainly quantified as a function of *remediation efficiency* through above mentioned methods for calculating each of them.

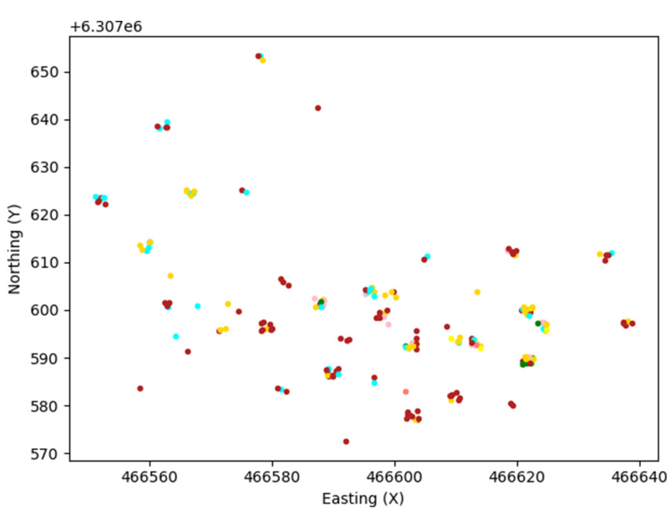


Fig. 4. K- means clustering output of all observation wells and all chemical parameters for 10 clusters.

Remediation efficiency is set to 0 for the time before 2020, as there was no remediation strategy in place, and to 1 when 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 periods (years) after 2020 when no option is chosen (Naseri-Rad et al., 2021), the efficiency of a strategy 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 (re)act accordingly. This lag, specified as the perception time, has been set to 2 years, and results in the evolution of the criterion as seen in Fig. 5b.

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. This is done because these factors are presumably higher when the remaining concentration in the recipient is higher and consequently more actions are needed to reduce it. Therefore, these four parameters are considered as the concentration at any time divided by the initial concentration and result in normalized values for all criteria. It should be noted that when concentrations are low, the criteria *exposure risk to humans* and *risk for secondary contamination* will be low (little to no risk exists). Thus, these criteria have been set to zero for concentrations below 100 μg/L, which is the remediation target.

Remediating action may be stopped after reaching the remediation target with an acceptable safety margin. There is always a risk for rebound (Fetter et al., 2018) and remediation action should last long enough to minimize that, while keeping the overall cost of the project reasonable. There are various approaches to long-term post remediation site management, which include engineering controls (ECs), long-term monitoring (LTM), institutional controls (ICs), and monitored natural attenuation (MNA) (Hou et al., 2020). These potential actions are not considered here, as only the treatment process is in focus. Instead, in this study, a concentration of 20 μg/L, which is one fifth of the remediation target, is considered as a suitable representation for this. It should be noted that this concentration limit needs to be site specific. For example, for a site with considerably more fine geologic material (which will enhance the rebound effect) or for sites with more exposure risk to humans, such limiting concentrations must be set to lower values. However, it should be noted that reaching these (very) low concentrations may take a much longer time and correspondingly higher budget, which would reduce their applicability. Thus, the model is set to run if the remaining concentration at the recipient is not lower than 20 μg/L. Remediation time continues to increase linearly, until remediating action is stopped, and capital cost is constant after the starting time of the action.

Finally, Fig. 6 depicts sustainability over time for the entire simulation, i.e., from the initial point when pollution occurs (Fig. 6a), as well as with focus on the management timeframe, i.e., starting time for the remediation scenarios (Fig. 6b). Notably, bioremediation may be the only remediation alternative that compensates the overall sustainability impacts in its life cycle (the sustainability plot goes back to 1); although it is not the most sustainable during the early years (having the steepest slope before 2030). On the contrary, more gentle measures like the base case (no additional strategies implemented) and MNA have the least overall sustainability, although they seemed initially to be the most sustainable options (see their mild slope compared to the other options before 2030). This is due to the fact that these require only a modest investment, do not generate large amounts of waste and emissions, and does not cause significant disturbance and health risk for residents and remediation staff (if handled in a standard way). If these measures could perform well and the remediation target was reached, they could get the highest sustainability scores; as recognized also in some previous studies (Hou, 2020; O'Connor and Hou, 2020; Onwubuya et al., 2009). However, remediation efficiency plays an important role, and in our case study such measures would not reach the remediation target within a suitable management timeframe of 30 years. Therefore, as the Fig. 6 shows, the passive approaches could not compete

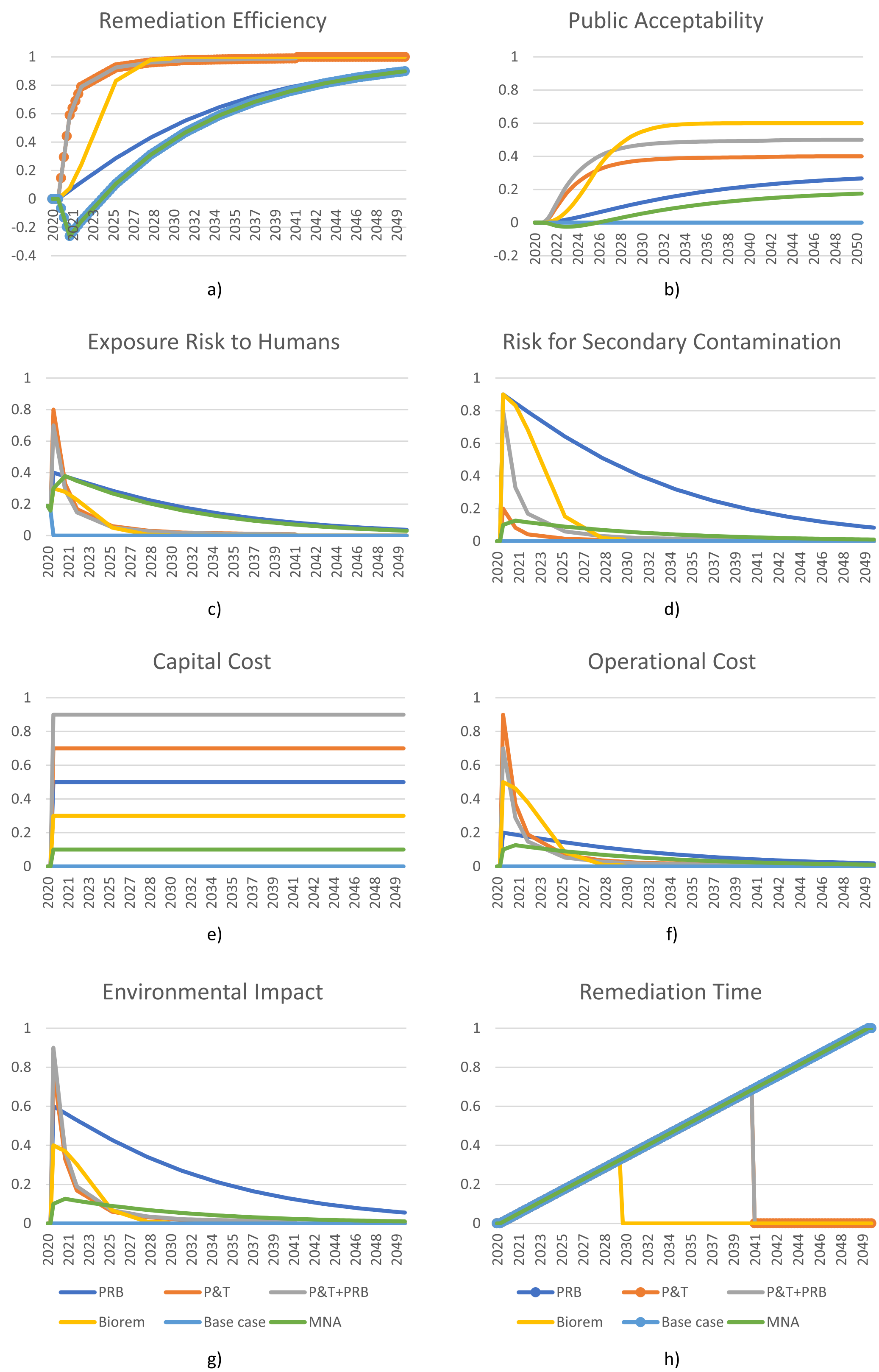
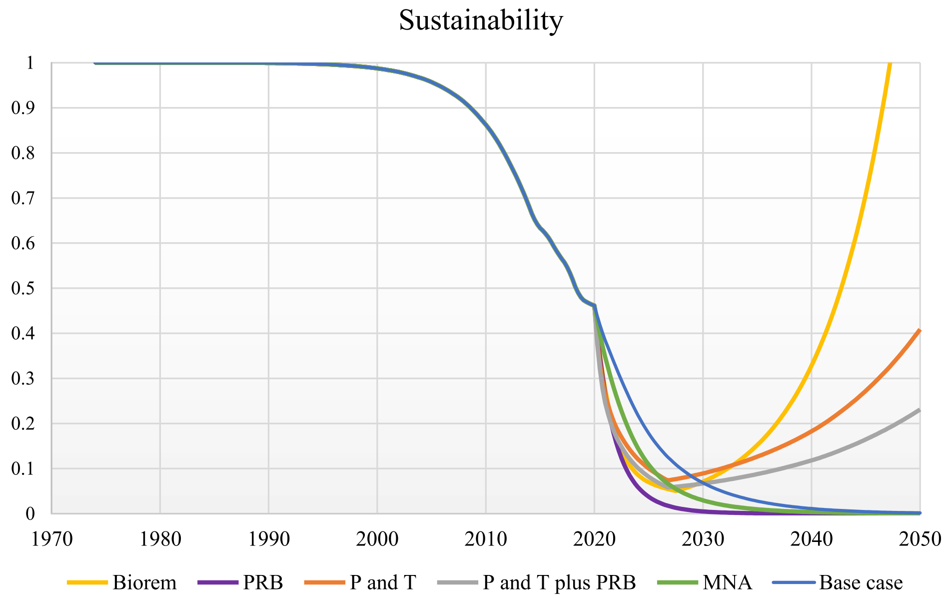
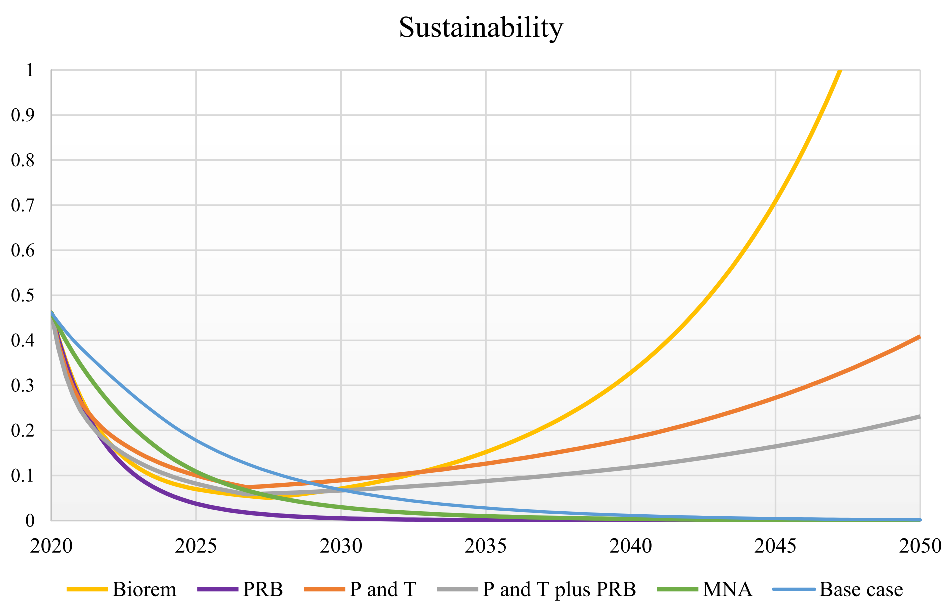


Fig. 5. Temporal change in each criterion for the 6 different scenarios. Horizontal axis in all plots represents years and the vertical axis shows sustainability of different remediation scenarios, normalized in a 0–1 scale (negative values are due to higher contamination concentrations compared with the starting point of remedy methods in 2020). Legends are the same for all plots and are provided in the end.

with more active measures in terms of overall sustainability, which include socio-economic considerations. These insights and the optimum possible use of such gentle measures versus more active measures are important results that DynSus can provide. As expected, measures requiring more actions are less sustainable at the early stage (except for the PRB), while compensating their overall sustainability score at the end.



A)



B)

Fig. 6. Sustainability of each scenario in time, A) from 1974 to 2050, B) from 2020 to 2050.

The biggest surprise, however, may be the low sustainability performance of PRB. PRBs are typically considered to be a sustainable method for the remediation of cases where the site-specific conditions and contaminant properties allow them to be effectively considered. As mentioned in Section 3, the geology of the site is characterized by glaciofluvial tills with a significant percentage of fine materials on top of a fractured bedrock. The PCP plume is found in various forms at the site in three phases: LNAPL, DNAPL, and dissolved in water. Moreover, the shallow groundwater table at the site, with a depth of about 1 m, may complicate the design of effective PRB structures. Considering these challenges, PRB might not be fully functioning at the site (Johansson, 2020) and that is why its decontamination rate, estimated by INSIDE-T, and consequently its overall sustainability performance over time are not desirable. This is an example for key insights that dynamic SA may provide, and which would have been otherwise neglected.

In summary, the model can simulate the dynamic behavior of governing parameters, which may be updated repeatedly based on observed concentrations and/or any pilot measures that occur at the site. In the same way, perceived scores for different criteria may change through the life cycle of a remediation project, affecting other criteria, as captured by the feedback structure of this DSS. This may accordingly change the whole system multiple times.

4.3. Decision making under uncertainty

High uncertainty associated with contaminant spread is intrinsic to contaminated sites modeling and consequently SA studies. This is acknowledged and shown in this study through the K-means clustering practice. However, it is important to note that SD models aim to enhance the understanding of complex systems and provide new insights of system behavior in time (Srijariya et al., 2008) and not necessarily predictions (Sterman, 2000). The use of INSIDE-T, and consequently DynSus, does not guarantee a certain contaminant concentration after several years at a certain location. Instead, such DSS tools are expected to improve the general understanding of the factors that may affect the entire remediation system and thus the degree of sustainability. Accounting for uncertainty of the decontamination process helps elucidate involved changes for different scenarios.

There are two main sources of uncertainty in the model INSIDE-T. One uncertainty stems from the site-specific transport parameters, where inverse modeling is used in INSIDE-T prior to predictive modeling 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 and used here as well. The other source of uncertainty in INSIDE-T is the assumed decontamination rates for the different remediation options. Although great care has been taken to arrive at reasonable assumptions using previous studies and estimations from experienced site managers, decontamination rates cannot be reliably assumed for many of these options and considering the potential for many different geologic settings. Complex hydrogeologic media induce high uncertainty of remediation performances even after performing pilot scale trials. Thus, the main aim here is to improve the overall understanding of the system's sustainability and consider additional factors that may not be typically assessed.

Nevertheless, to further demonstrate DynSus capabilities regarding accounting for uncertainty, we introduced a perturbation of ±10% on assumed decontamination rates in all scenarios. Fig. 7 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.

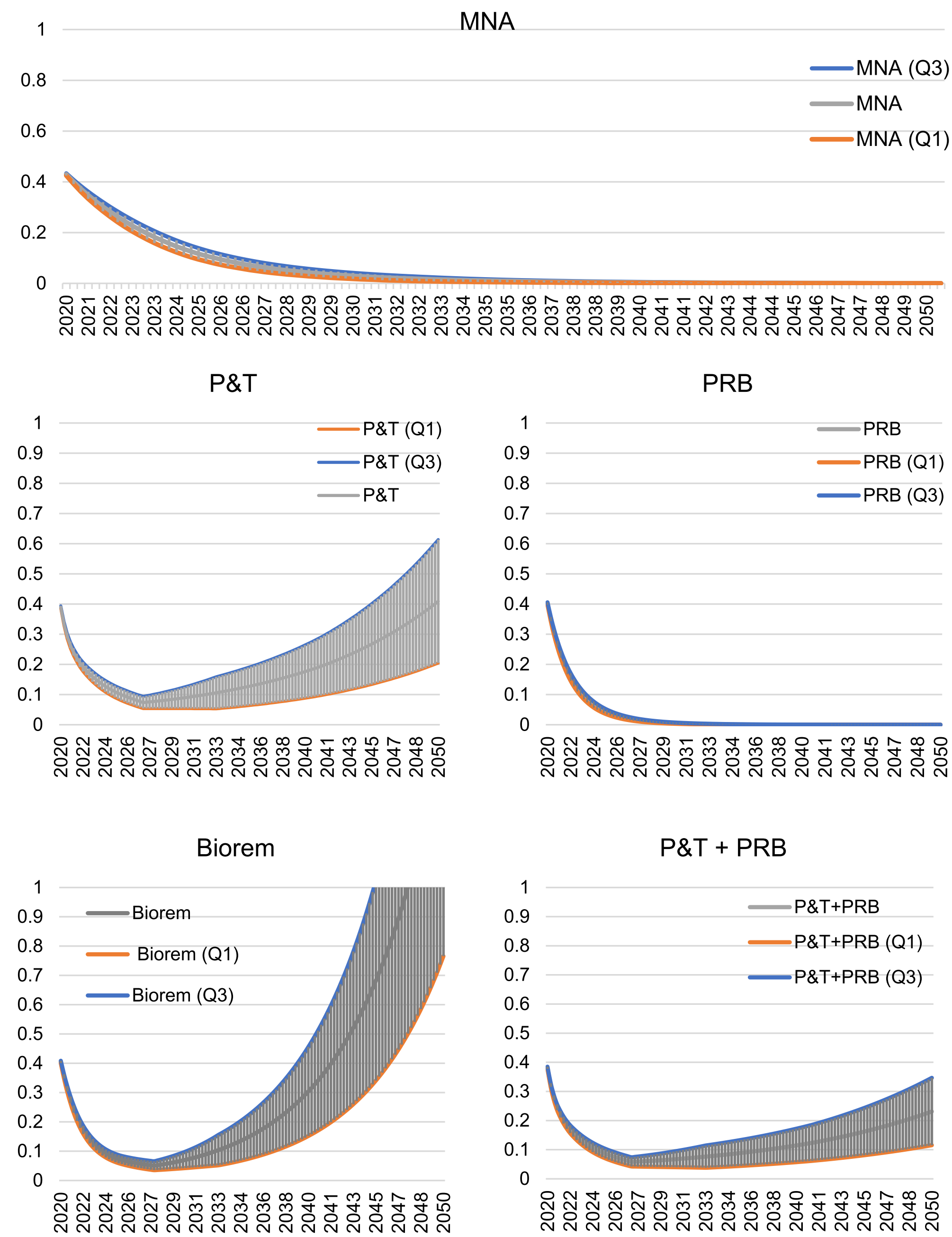


Fig. 7. Temporal uncertainty progression for the final sustainability scores for different remediation options resulting from a 10% perturbation in the transport parameters for INSIDE-T. Orange and blue lines represent modeling results through applying 1st and 3rd quartiles of transport parameters values, respectively.

The results, as illustrated in Fig. 7, 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. Nevertheless, these results may help and encourage managers to improve other aspects of the system for more sustainable actions. For example, in the case that P&T is selected as a remediation technology, its sustainability may be improved by reducing the scores of negative criteria, such as *environmental impacts* (e.g., by consuming more clean energy or better handling of the generated waste), which would improve its overall sustainability results. Fig. 7 does not indicate significant uncertainty in the starting years of remedy actions. Except for scenarios that are not likely to reach the remediation target in 30 years, most of the uncertainty results during later years.

Finally, the life cycle perspective of sustainability dynamics for our 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). Such models for real world problems are, however, just simple representations of the remedy measures, and that further studies into its particular aspects still 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 criteria. The combination of P&T and PRB and the PRB alone did not show promising results, although the former showed good contamination removal capabilities.

5. Conclusion

In this study we integrated an efficient contaminant fate and transport model (INSIDE-T) with an SA tool for site remediation practice (INSIDE) via a system dynamics framework, creating the DSS DynSus. We then used this tool for evaluating the sustainability of multiple remediation scenarios. This integration helps 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 to deal with these.

Remediation efficiency is a key issue and driving factor in the dynamic SA of remediation scenarios. This criterion was thus used to integrate the predeveloped fate and transport model with the SA tool. However, these efficiencies are subject to change due to complex and heterogenic conditions of the subsurface environment. This necessitates a frequent updating of the model and considering the associated uncertainties. Notably, this method provides a transparent framework that lets site managers update each scenario coefficient as needed, after each field campaign, which will then impact the other criteria according to the defined interrelations (feedback structure of the SD model).

Some limitations need to be considered in the study. Firstly, although a SA needs some degree of subjectivity to incorporate all the aspects and DynSus is not an exception in this matter, this subjectivity must be treated with considerations. Only experienced site managers may be asked for scoring the remediation alternatives (assigning scenario coefficient). Secondly, 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 for 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. The assumption is that all alternatives presented here are feasible and only differ in their efficiency.

The present methodology provides an important holistic view for incorporating more robust data in view of different aspects (environmental, social, and economic) and methods to quantify them. Quantifying these aspects may lead to more reliable results by DynSus, 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 to this more general one. Applying DynSus for more sites may help in this regard.

CRediT authorship contribution statement

Mehran Naseri-Rad: Conceptualization; Data curation; Formal analysis; Funding acquisition; Investigation; Methodology; Project administration; Resources; Software; Validation; Visualization; Roles/Writing – original draft; Writing – review & editing.

Ronny Berndtsson: Resources, Conceptualization, Writing - Review & Editing, Supervision

Amir Aminifar: Data curation; Formal analysis; Visualization; Writing – review & editing

Ursula S. McKnight: Methodology; Writing – review & editing

David O'Connor: Writing – review & editing

Kenneth M Persson: Conceptualization, Writing - Review & Editing

Declaration of competing interest

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

Acknowledgement

This research was mainly funded by Ministry of Science, Research and Technology of the Islamic Republic of Iran, which provided the scholarship to the main author; it is also partly funded by *Åke och Greta Lisshed* foundation (Reference ID: 2021-00166), and *Hans Werthén Fonden*. The APC was funded by the Division of Water Resources Engineering, Lund University, Sweden. Also, WASP Program by the Knut and Alice Wallenberg Foundation provided funding for A. Aminifar. This research was not possible without kind support from Kristin Forsberg at Swedish Geological Survey (SGU), providing investigated site data.

Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.scitotenv.2022.154992.

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