Improving hydrogeological characterization using groundwater numerical models and multiple lines of evidence

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2024

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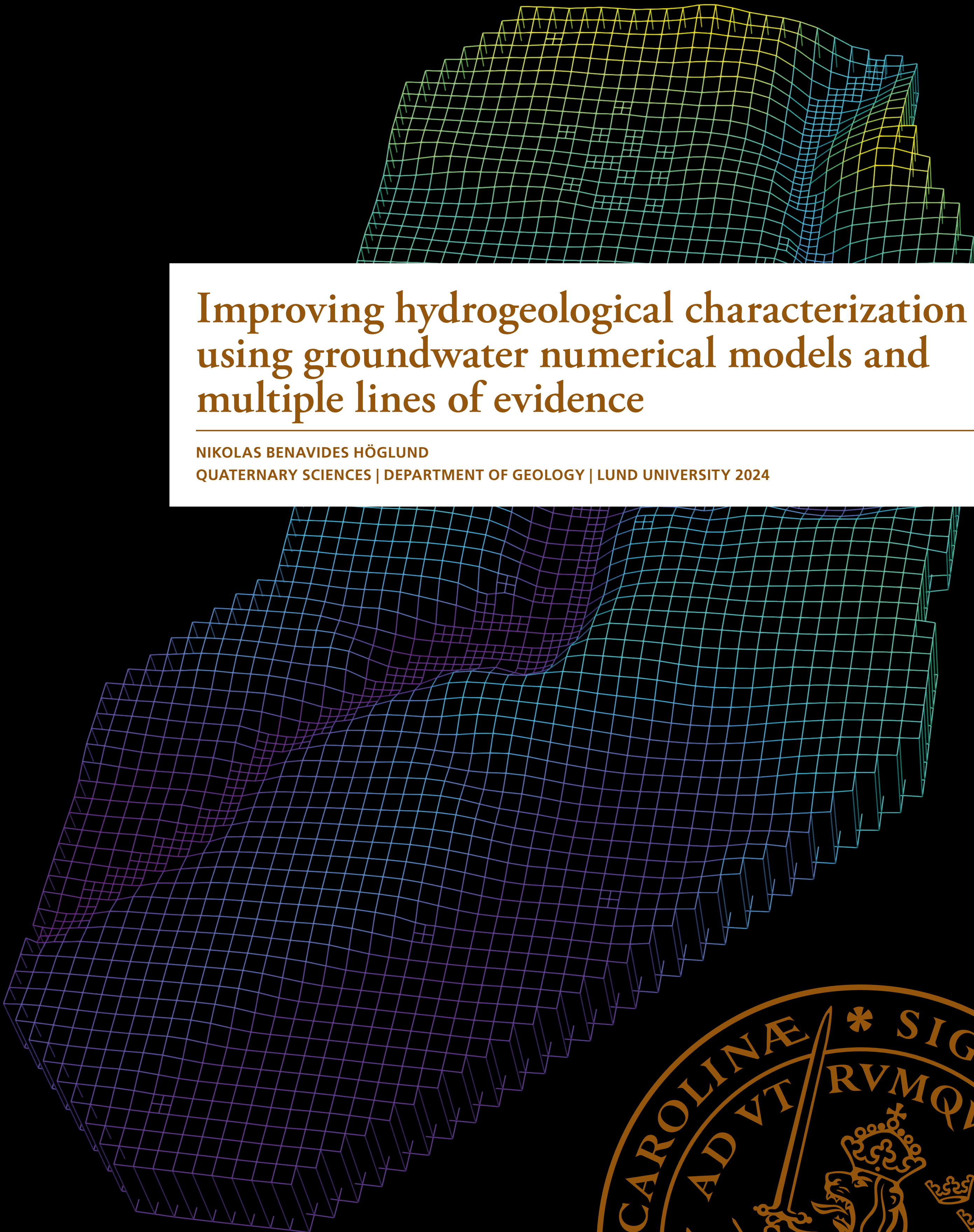
LUNDQUA THESIS 97



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QUATERNARY SCIENCES | DEPARTMENT OF GEOLOGY | LUND UNIVERSITY 2024

Printed by Media-Tryck, Lund 2024 NORDIC SWAN ECOLABEL 3041 0903

Quaternary Sciences
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Sölvegatan 12
SE-223 62 Lund, Sweden
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ISSN 0281-3033
ISBN 978-91-87847-84-4

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LUND UNIVERSITY

DOCTORAL DISSERTATION

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To be defended in Pangea, Geocentrum II, Sölvegatan 12
on the 6th of September 2024, at 09:15.

Faculty opponent
Prof. Karsten Høgh Jensen
University of Copenhagen

Cover image, front: Nikolas Benavides Höglund; back: Sofia Åkesson

Quaternary Sciences
Department of Geology
Faculty of Science

ISBN 978-91-87847-84-4 (print)
ISBN 978-91-87847-85-1 (pdf)
ISSN 0281-3033

Printed in Sweden by Media-Tryck, Lund University, Lund 2024

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MADE IN SWEDEN

<table>
<tr><td colspan="2" rowspan="2">Organization
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Department of Geology
Sölvegatan 12
SE-22362, LUND
Sweden</td><td colspan="2">Document name

DOCTORAL DISSERTATION</td></tr>
<tr><td colspan="2">Date of issue: August 15, 2024</td></tr>
<tr><td colspan="2">Author: Nikolas Benavides Höglund</td><td colspan="2">Sponsoring organization</td></tr>
<tr><td colspan="4">Title and subtitle: Improving hydrogeological characterization using groundwater numerical models and multiple lines of evidence</td></tr>
<tr><td colspan="4">Abstract

Groundwater is Earth's largest liquid freshwater resource. It is a significant component of the hydrological cycle and a buffer that sustains rivers and freshwater-dependent ecosystems during droughts. Approximately half of the world's population depends on groundwater for drinking water, food, and hygiene. It is used extensively in agricultural irrigation, food production and for industrial processes. However, pollution and over-exploitation pose serious risks to its sustainability, representing a global problem manifested on a local scale. Therefore, the responsible management of groundwater is critical to ensure its quality and availability for future generations.

Informed decision-making on groundwater management requires the underground, i.e. the material in which groundwater is stored and through which it flows, to be characterized. This thesis focuses on how this characterization can be improved by using groundwater numerical models as a framework for assimilating diverse types of data, including direct and indirect measurements of groundwater and underground properties, as well as expert knowledge. The scope of this thesis is twofold. Firstly, it investigates the extent and manner in which groundwater numerical models are currently applied within the industry to solve groundwater-related problems, as analyzed through the current state of the art in decision-support modelling. For practical reasons, this investigation focuses on applications in Sweden, but highlights insights applicable in an international context. Secondly, it explores methods for improving hydrogeological characterization through the assimilation of conventional and unconventional data types, with a focus on contaminated sites. These data types are then evaluated in terms of their contribution towards reducing the uncertainty of model predictions, providing insights on the value of information.

The findings highlights a significant gap between important academic advances in groundwater modelling and practical application within the industry, tracing this discrepancy to a lack of inclusion of concepts such as data assimilation and uncertainty quantification in groundwater education. Suggestions for improvement are presented, which include the formulation of flexible guideline recommendations for practitioners and the inclusion of aforementioned concepts in groundwater education. Additional findings highlights the high value of unconvential data, demonstrating that, depending on the model prediction, they can be as valuable as conventional measurements of hydraulic head or more. This likely challenges the prevailing line of thinking within the industry, but also presents an opportunity for improved modelling workflows among practitioners willing to embrace new concepts. This thesis presents tangible examples for how this can be achieved in order to improve hydrogeological site characterization, demonstrated using transparent and reproducible model workflows of two contaminated sites in Sweden.</td></tr>
<tr><td colspan="4">Key words: groundwater, groundwater modelling, contamination, parameter estimation, data assimilation, uncertainty analysis</td></tr>
<tr><td colspan="4">Classification system and/or index terms (if any)</td></tr>
<tr><td colspan="3">Supplementary bibliographical information</td><td>Language: English</td></tr>
<tr><td colspan="3">ISSN and key title: 0281-3033 LUNDQUA THESIS</td><td>ISBN: 978-91-87847-84-4</td></tr>
<tr><td rowspan="2">Recipient's notes</td><td colspan="2">Number of pages: 137</td><td>Price</td></tr>
<tr><td colspan="3">Security classification</td></tr>
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Signature: Date: 2024-06-27

"We demand rigidly defined areas of doubt and uncertainty!"
— Douglas Adams, The Hitchhiker's Guide to the Galaxy

Contents

List of papers

This thesis is based on the following publications and manuscripts:

Paper I

Groundwater Modelling for Decision-Support in Practice: Insights from Sweden
Benavides Höglund, N., Sparrenbom, C., & Barthel, R. & Haraldsson, E. (2024).
Submitted to *Ambio*. Accepted with minor revisions (June 2024). Under revision.

Paper II

A probabilistic assessment of surface water-groundwater exchange flux at a PCE contaminated site using groundwater modelling
Benavides Höglund, N., Sparrenbom, C. & Hugman, R. (2023).
Frontiers in Earth Science, 11, https://doi.org/10.3389/feart.2023.1168609

Paper III

Multidisciplinary Characterization of Chlorinated Solvents Contamination and In-Situ Remediation with the Use of the Direct Current Resistivity and Time-Domain Induced Polarization Tomography
Nivorlis, A., Dahlin, T., Rossi, M., Höglund, N. & Sparrenbom, C. (2019).
Geosciences, 9, https://doi.org/10.3390/geosciences9120487

Paper IV

Assimilation and Worth of Injection Response Data for Enhanced Contaminated Site Characterization
Benavides Höglund, N., Sparrenbom, C. & Hugman, R. (2024).
Submitted to *Hydrogeology Journal*. Accepted with minor revisions (April 2024). Under revision.

Acknowledgments

First, I want to thank you, my supervisor, Charlotte Sparrenbom, for your support and encouragement during this project. Your supervision provided me with the freedom to explore and learn on my own, but also challenged me when necessary. This provided a good balance that promoted my growth, kept me on the right path, and enhanced my ability for scientific research.

Rui Hugman, thank you for agreeing to join us on this project as my co-supervisor. Your expertise in modelling came at a critical time and your support greatly improved my work.

Sven Lukas, thank you for being my co-supervisor here at the department, knowing I could consult you if needed was a great comfort. Thank you also for your valuable feedback on this thesis.

I'm grateful for being part of the MIRACHL research group. Our collaboration in the field, along with our discussions and joint interpretation sessions, broadened my understanding of the different aspects of contaminated site characterization. A special thanks to my fellow Ph.D. students within our project, Sofia Åkesson and Aristeidis Nivorlis. I spent some of my most memorable times in this project with you, hauling equipment across the country and enduring rainy, cold, and dark Swedish nights in the mud, taking measurements and samples. Somehow, this climate was preferable to the warm and sunny days when temperatures turned the hazmat suit and facemask into a sauna, and doing precision work while fighting off claustrophobia became a mental battle. Julia Björn and Jessica Jennerheim, thank you for your efforts during the long hours of fieldwork. Of course, Charlotte, Torleif Dahlin, Matteo Rossi, Catherine Paul, and Tina Martin, the support you showed us Ph.D. students during these years is greatly appreciated.

Roland Barthel, thank you for joining us in our work focusing on decision-support modelling in Sweden. Together, we wrote the paper I wished had existed when I first started my Ph.D. candidacy. Ulf Winnberg and Kristin Forsberg at SGU, I'd like to thank you both for our collaboration on the contaminated site in Hagfors. John Doherty, thank you for providing me with the source code and instructions for compiling PEST in Linux environments. This allowed me to utilize the university's high performance computing cluster, saving me countless hours. Thank you also for the great work you've contributed to our field over the years, including many of the tools which I used to perform my analyses. Jonas Lindemann, Anders Follin and Marcos Acebes, thank you for your support with the LUNARC systems.

Ethan Silvester and Ida Lunde Hygum, my fellow Ph.D. students with whom I share the office. Thank you for all our interesting conversations over the years and I wish you both the very best in the future.

To my fellow Ph.D. students at the department, I'm sorry for missing out on the many events that were organized over the years. The few events that I attended, I enjoyed very much. To you and all other colleagues at the department, I want to say a heartfelt thank you for the time I've got to share with you and for the valuable feedback you've provided me with during seminars and presentations.

This project would not have been possible without the funding provided by the Swedish Research Council (ref. 2016-20099 and ref. 2016-00808), SBUF (ref. 13336 and 13938), the Swedish Geological Survey, ÅForsk (ref. 14-332), NCC, Sven Tyréns Stiftelse, the Royal Physiographic Society (ref. 40844), Landshövding Per Westlings minnesfond (ref. 2023-0029) and Lund University. In addition, I would like to specifically acknowledge the Swedish taxpayers for enabling this research. It is my sincere hope that this work will, at the very least, make a small contribution towards more informed decision-making regarding our shared freshwater resources. Thank you.

Mi querido padre, a quien trágicamente perdí durante este tiempo, sé que estarías orgulloso. Te extraño mucho. Kära mor, tack för allt ditt stöd. Äntligen blev jag klar! Rikard, kära bror, tack för alla samtal under åren. Till resten av min familj och alla goda vänner, tack för ert stöd.

Ida, Sam, Siri och lilla Björn. Ni är det finaste jag har.

Lund, June 2024

Nikolás Emilio Benavides Höglund

1 Introduction

Water covers most of our planet's surface and is essential for life on Earth (e.g., Westfall & Brack, 2018). The distribution of water is uneven across the planet, and occurs in gaseous, liquid, and solid phases. The hydrological cycle describes the movement of water between the different phases across the lithosphere, atmosphere- and biosphere, driven by gravity and solar energy, through processes such as evapotranspiration, condensation, precipitation, infiltration, and runoff. Most of Earth's water is saline and resides in the oceans (> 97 percent; e.g., Stephens *et al*., 2020). Of the remaining freshwater, approximately 77 percent reside in glaciers and icecaps, most of which (> 85 percent; Huss & Farinotti, 2012) are located in sparsely-populated regions, including Antarctica, Greenland, Arctic Canada and Siberia. Available liquid freshwater, essential for terrestrial life and ecosystems, consists mainly of groundwater (98-99 percent; e.g. UNESCO, 2022). Most surface water, such as rivers and lakes visible to the human eye, are sustained by groundwater discharge, which acts as a buffer to prevent them from drying out (Winter *et al*., 1998; Woessner, 2020).

Although groundwater is the most abundant freshwater resource, it is comparatively more difficult to extract than surface waters, especially from a historical perspective. This has put many of the planet's surface waters under stress as human activities have expanded, posing risks to public health and ecosystems (WHO, 2016). Moreover, competition for surface water resources, especially in areas of scarcity, can be a driver for conflict (Schillinger *et al*., 2020), increasing the likelihood of surface waters being used as a weapon or targeted during conflicts (Gleick, 2019). Today, groundwater abstraction accounts for approximately half of the world's domestic freshwater use and more than 40 percent of water used for irrigation (Siebert *et al*., 2010; Margat & Van der Gun 2013), highlighting the critical role of groundwater in meeting global freshwater demands (Scanlon *et al*., 2023; World Bank Group, 2023). Compared to surface waters, groundwater, especially when infiltrating and flowing through unconsolidated porous media, tends to be of higher quality, as harmful bacteria and viruses are filtered out through mechanical and microbiological processes in the sediments (Robertson & Edberg 1997; Sen, 2011. However, despite its abundance and generally higher quality, serious threats to both the quantity and quality of groundwater can be identified. These include depletion in areas where abstraction exceeds natural recharge rates at local and regional scales around the globe (Giordano, 2009; Wada *et al*., 2010; Jasechko *et al*., 2024), degradation of water quality due to human expansion and the introduction and accumulation of pollutants, including 'forever chemicals' such as PFAS (Fienen & Arshad, 2016; Brunn *et al*., 2023).

Groundwater forms as precipitation and surface water infiltrates into and through the unsaturated zone ultimately reaching the saturated zone where all void space is saturated with water. This process can take hours to months, depending on the geological settings (Horton, 1933; Bodman & Colman, 1944). The residence time of groundwater also varies widely (Fig. 1), and typically ranges from decades in highly-conductive glaciofluvial deposits (e.g., Boucher *et al*. 2015), to centuries in shallow bedrock and sedimentary aquifers (e.g., Åkesson *et al*. 2015), to millennia or even millions of years in deep sedimentary aquifers (e.g., Sturchio *et al*. 2004). Developing an understanding for the disposition of the subsurface, which is unique to each site's geological setting, is critical for the understanding of the groundwater system and for responsible groundwater management at local and regional scales (e.g., Mackay *et al*, 1986; Enemark *et al*, 2019). This process, often referred to as 'hydrogeological characterization', is essential for assessing issues relating to groundwater quantity, quality, and mobility.

A variety of methods can be employed for characterization purposes, including drilling boreholes for stratigraphic logging and sample collection of both water and sediments, performing aquifer tests, tracer studies, direct-push probing, or non-intrusive surface geophysical measurements and so on. These methods contribute to developing conceptual and process-based numerical models of the subsurface. If uncertainties related to the properties of the subsurface are to be considered, as they often should (Gómez-Hernández, 2006), data gathered with these various techniques can be used to construct a stochastic representation of the subsurface. Such an approach could consist of multiple, equally probable, realizations of underground properties that govern the quantity, quality and mobility of groundwater and substances therein. Using groundwater numerical models, these realizations can be assimilated with a comprehensive set of measurements of past system behaviour, such as e.g. records of groundwater level (head), groundwater chemistry and stream flow rates. These integrations can enhance the robustness of the decision-support model, potentially aiding decision-makers in developing sustainable groundwater management plans (Ferré 2017; Doherty & Moore, 2020).

In this context, an area that has seen extensive use of groundwater numerical models is the management of contaminated sites. Although these sites may present threats to public health and ecosystems at local and regional scales, their widespread occurrence is a

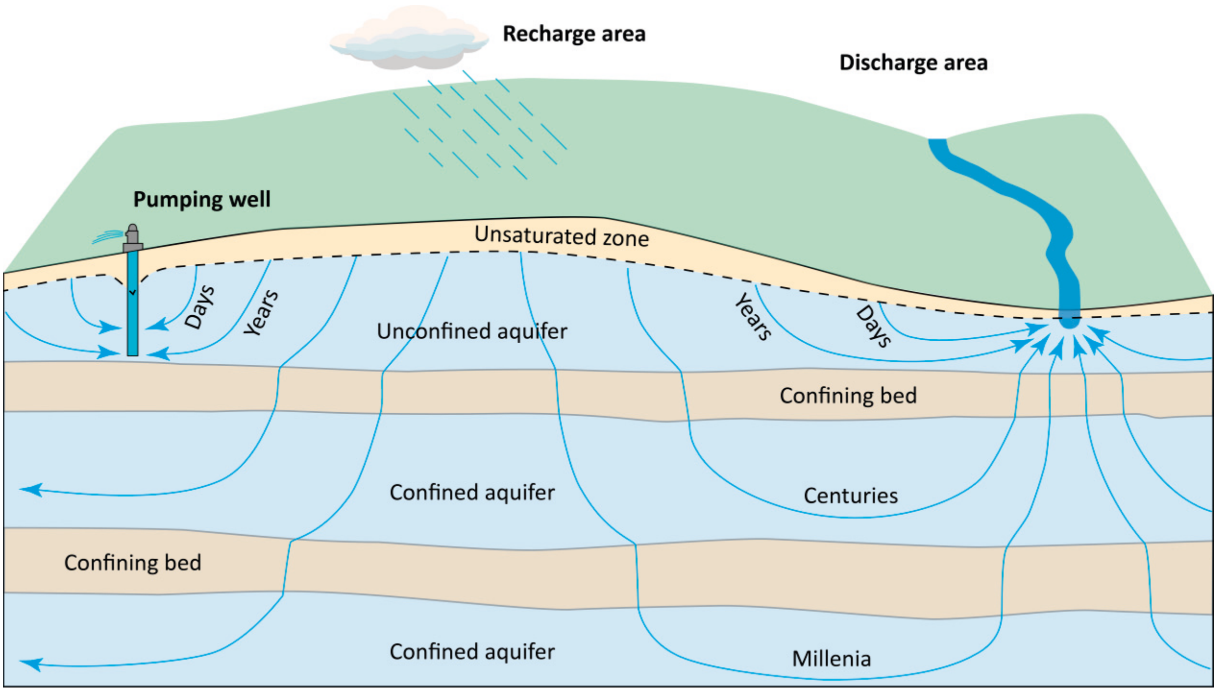

Figure 1. Illustration showing the formation of groundwater through precipitation and recharge, groundwater flow paths and residence times in heterogeneous media, and its discharge into a stream and extraction via pumping. Adapted from Winter *et al.* (1998).

global problem (Sinnett *et al*., 2022). Groundwater numerical models can serve to quantify and predict the outcome of different management actions, such as various treatment strategies, thereby providing decision-makers with insights into the most suitable approaches for mitigating contamination (Anderson *et al*., 2015). However, to do so effectively they should be viewed as decision-support tools rather than mere simulations of groundwater flow (e.g. Benavides-Höglund *et al* 2023, Paper I in this thesis). This implies that data assimilation and uncertainty analyses are considered integral components of a modelling workflow, complementing simulation (Doherty and Moore, 2020). Such workflows ensure that any such model is both informed by historical measurements, and that predictive uncertainty is quantified. In the context of contaminated site management, this means that ancillary observations such as aquifer test response, expert knowledge, and groundwater chemistry, of which plenty often exist for these sites and which may include direct or indirect information relevant to the outcome of a remediation action, should be assimilated. These observations should be combined alongside historical measurements of the system's state, such as water levels and flow rates, to reduce predictive uncertainty.

This thesis and the papers presented herein elaborate on groundwater numerical modelling for site characterization and decision support, with an emphasis on contaminated sites. In particular, a key aim is to investigate how different types of observations (multiple lines of evidence) can be assimilated into the modelling framework to improve the robustness of workflows and reduce predictive uncertainties. To put this subject into a wider context, education and its application within the industry is also explored. The work involves the integration of a multitude of different data sources assimilated across disciplines, including: Quantitative and qualitative information collected in the field and from digital repositories; multidisciplinary fieldwork conducted at two contaminated sites in Sweden; and numerical modelling utilizing a high-performance computing (HPC) cluster at Lund University. In addition to the scientific findings presented herein, the outcomes of this thesis may serve to shape future education on this topic and inform stakeholders and the industry about concepts widely employed in academia but less so in practical applications, thereby helping to bridge this gap.

2 Scope of the thesis

This thesis focuses on the characterization of groundwater systems through the assimilation of both conventional and unconventional data. This includes direct measurements of system states and synthetically engineered datasets from these measurements (hard data), along with information derived from expert knowledge (soft data). The objective is to explore how ancillary observations, not typically part of traditional groundwater modeling workflows, can be integrated to improve the robustness of model assessments, ultimately leading to better-informed decision-making on vital freshwater resources. Furthermore, it investigates the current application of groundwater numerical models in addressing water-related issues within the industry as well as how this is delt with within the educational sector, providing a baseline from which insights into possible gaps and opportunities can be identified. For reasons of feasibility, this latter investigation focuses on applications in Sweden, yet considers its implications and potential applicability across broader regional and international contexts. More specifically, the work included in this thesis aims to:

1. Investigate the use of groundwater numerical models across industry sectors, their assessment objectives, and the relationship between industry methods, education, and academic research;
2. Explore how conventional groundwater data can be coupled with unconventional data and local expert knowledge to characterize surface water-groundwater exchange flux;
3. Develop methods for improving site characterization by assimilating information on aquifer response to injection events (injection-response data); and
4. Quantify the worth of injection-response data in terms of reducing parameter uncertainty.

3 Background

While this chapter provides a background on contaminated sites and hydrogeology in general, and groundwater modelling in particular, it should be noted that these subjects are broad and can be approached from many different angles, all of which cannot possibly be covered in this thesis. Therefore, the focus of this chapter is to provide background specific to, and most relevant for, the concepts and research presented in this thesis. Readers seeking further elaboration on specific topics are encouraged to refer to the cited literature and beyond.

3.1 Groundwater contamination and chlorinated solvents

Contaminated groundwater poses a serious hazard to our ecosystems and human health, and direct exposure or intake can cause severe negative impacts both at the individual level and for the overall health of communities (WHO, 2011). There is also a strong economic incentive to prevent contaminants from polluting groundwater because remediation or substitution of freshwater resources comes at a great cost (e.g., Dodds *et al*., 2009; Cordner *et al*., 2021).

Landfill, pesticide and road salt leachates, leaking storage tanks and septic systems, acid mine drainage and chemical spills are examples of some of the most common sources of groundwater contamination (Fetter, 1999; Swartjes, 2011). Depending on the properties of the contaminant and the geological material, contaminants may dissolve, degas, sorb, react or remain in free phase. Hydrophobic, free-phase contaminants, often termed NAPL (non-aqueous phase liquid), vary in behavior based on their density. If lighter than water (LNAPL), they may pool on top of the groundwater. If denser than water (DNAPL), they sink through the water column and rest or slowly flow according to the overall surface gradient on a confining layer (Pankow & Cherry, 1996). Contaminants that dissolve in water may diffuse into the matrix of the subsurface and adsorb to particles, contributing to the formation of complex plumes that evolve over time, depending on the relative importance of advection, dispersion, and reaction processes. Determining the disposition, properties and behavior of contaminants requires sampling and characterization of the subsurface.

Guideline values for many chemical compounds and microbiological contaminants have been established by various organizations, including the Swedish Environmental Protection Agency (SEPA, 1999), U.S. Environmental Protection Agency (U.S. EPA, 2009) and WHO (2017). In Sweden, guideline values for drinking water are established by the Swedish Food Agency (Livsmedelsverket, 2001; 2017), and for groundwater quality by the Swedish Geological Survey (SGU, 2013), the latter of which is the authority responsible for the national environmental quality objective 'Good-Quality Groundwater'. Additionally, the SEPA (2022) establishes guideline values for contaminated soil. Presence of contaminants above guideline values marks a potential risk to public health and environmental safety, necessitating assessment and appropriate remedial actions to ensure the sustainability of groundwater resources.

In Sweden, the assessment process of potentially contaminated sites is guided by a model referred to as the Method for Inventory of Contaminated Sites, established by SEPA (1999) and abbreviated MIFO (Metodik för Inventering av Förorenade Områden) in Swedish. The MIFO model divides the assessment of a suspected contaminated site into two phases: Initially, an overview study leads to a preliminary risk categorization across four levels, with Level 1 indicating the highest risk. Subsequently, for sites categorized as Levels 1 through 3 in the initial study, a more detailed investigation is performed, involving broader sampling efforts to verify or revise the initial risk assessment. After the second phase of investigation, sites categorized as Level 1 or 2 are prioritized for further investigation and remediation. According to SEPA (2024), as many as 86 000 potentially contaminated sites exist in Sweden alone, highlighting the urgency to mitigate further contamination as well as to treat known contaminations.

Multiple approaches exist for remediating contaminated sites, involving both ex-situ and in-situ solutions. Typically, the preferred approach for the remediation of contaminated sites is in-situ, as it is considered safer from both health and environmental perspectives because transporting contaminants increases the risk of exposure and may introduce them to new areas, posing additional risks of pollution. Several techniques for in-situ remediation of contaminated ground and groundwater have been developed over the years. Some of the most common include pump-and-treat systems, plume containment barriers, vapor extraction, thermal remediation, air sparging, bioslurping and the injection of remediation fluids, or a combination of these techniques (Fetter, 1999; Swartjes, 2011). Choice of technique is typically influenced by the available budget, type of contaminant, geological setting, remediation target and any additional factors to consider, such as e.g. nearby buildings and infrastructure.

Chlorinated solvents are common groundwater contaminants (Pankow & Cherry, 1996). They are a group of chemical compounds typically used in dry cleaning and metal-degreasing processes for their effectiveness in dissolving organic materials. Chlorinated aliphatic hydrocarbons constitute a subgroup of chlorinated solvents that are hydrophobic and denser than water (DNAPLs) and are characterized by two double-bonded carbon molecules with chlorine replacing one or more hydrogen atoms, depending on the specific compound. Tetrachloroethene (PCE) is the primary compound and may degrade into its metabolites trichloroethene (TCE), cis-1,2-dichlorothene (cis-DCE), vinyl chloride and ethene (Pankow & Cherry, 1996; Wiedemeier, 1999) through stepwise replacement of chlorine atoms with hydrogen (Fig. 2). Exposure to chlorinated solvents, specifically TCE and vinyl chloride, is known to cause cancer in humans, with PCE and cis-DCE being suspected of causing cancer in humans (U.S. EPA, 2000; Wartenberg *et al*., 2000; Guha *et al*., 2012). Occurrences of these compounds as contaminants in soil, bedrock and groundwater are often concentrated in industrial areas where they are spilled and infiltrate into the ground. However, due to the slow natural degradation of chlorinated solvents, they can also be found as remnants in areas historically used by industries and dry-cleaning facilities, highlighting the importance of understanding a site's historical context, as these contaminants can remain underground for many years. Once free-phase PCE infiltrates into the ground, it tends to sink through the soil and groundwater column, ultimately pooling on impermeable or semi-impermeable surfaces such as crystalline bedrock or clays, or accumulating in fractures (Pankow & Cherry, 1996). Over time, PCE may dissolve in groundwater and be transported through advective flow or diffuse into the fine-grained matrix of the soil and bedrock, where it can persist for many years. This persistence contributes to the continued spread of PCE and its metabolites through back-diffusion processes (Chapman & Parker, 2005; Chapman *et al*., 2012), rendering it difficult to remediate via pump and treat actions.

Common techniques for remediating PCE and its metabolites include thermal remediation and enhanced natural attenuation, both of which typically involve underground injections. In thermal

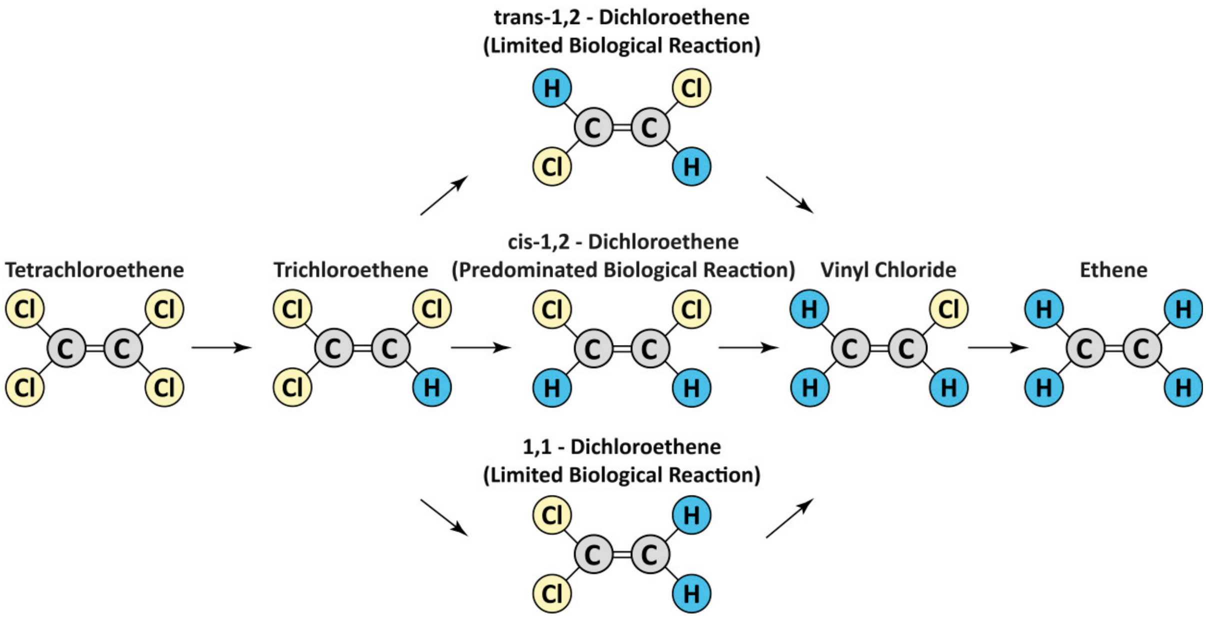

Figure 2. Stepwise degradation sequence of chlorinated aliphatic hydrocarbons from tetrachloroethylene (PCE) to ethene, adapted from Wiedemeier (1999). Degradation can occur naturally or can be accelerated through the use of enhanced degradation methods.

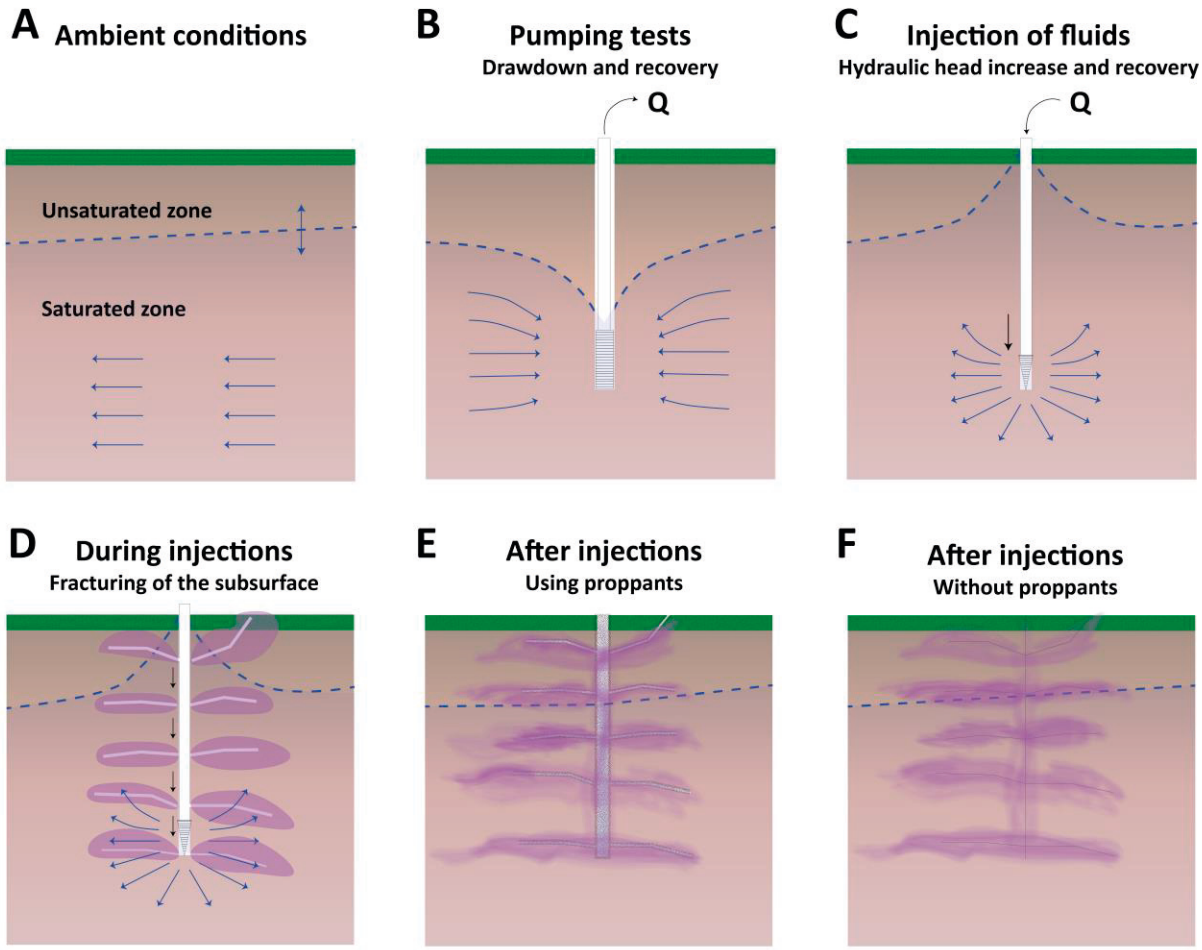

Figure 3. The hydrogeological setting under varying conditions, including A) naturally varying ambient conditions, B) drawdown of hydraulic head due to pumping, and C) increase in hydraulic head due to injection of fluids under conditions that does not fracture the underground. D) shows hydraulic fracturing of the subsurface due to high injection pressures, E) and F) display dissolution and transport of amendments after injections under permanently (E) or temporarily (F) increased permeability.

remediation, pipes are drilled into the source zone, and steam injections or electrical heating cause the contaminant to vaporize (e.g., Parkinson *et al*., 2004). This vapor is then extracted from the underground and filtered through a carbon filter. Heat injections can provide effective treatment of source zones (e.g., Baker *et al*., 2016), but they are also associated with considerable costs due to the infrastructure and energy required for heating the subsurface and capturing the vapor. In enhanced natural attenuation and bioremediation, fluids containing nano zerovalent iron (nZVI) or a combination of a carbon source and bacterial consortium are introduced into the contaminated soil to enhance natural degradation processes (Fig. 2; e.g., Schneidewind *et al*., 2014; Sheu *et al*., 2016). For effective natural degradation of chlorinated solvents, the underground conditions should be reducing (anaerobic), and the appropriate type of microorganisms should be present, along with an energy source to fuel microbial metabolism (NRC, 1993), such as molasses or emulsified vegetable oil. Amendment fluids carrying nZVI particles contribute to enhancing these reducing conditions by acting as electron donors and facilitating reductive dechlorination. Additionally, or alternatively, dehalogenating bacteria capable of complete stepwise degradation of PCE to ethene (Löffler *et al*., 2013) may be injected with nutrients to initiate or enhance the microbial degradation of PCE. The delivery methods of amendments can also influence the distribution of remediation fluids and its effectiveness underground. Although typically associated with the petroleum industry, hydraulic fracturing has become an established method in environmental engineering for delivering amendments (e.g., Murdoch, 2002), as it increases the surface area for reactants to interact (Fig. 3). Other common injection techniques include direct-push delivery for contaminants in shallow, unconsolidated media and gravity injection into existing wells (e.g., Christiansen *et al*., 2012; Comba *et al*., 2011).

3.2 Groundwater flow in porous media

Groundwater flowing through the subsurface is typically described using Darcy's (1856) Law, which describes saturated laminar flow of fluids through porous media. However, not all media in which groundwater flows are best described as porous. In settings involving flow through karstic systems or

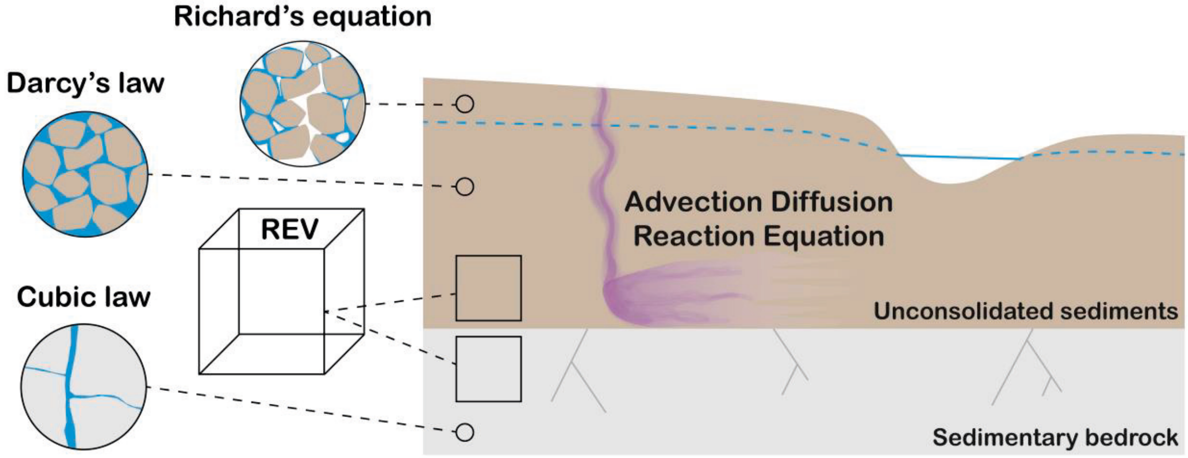

Figure 4. Governing theory of groundwater flow and solute transport in relation to different hydrogeological settings and scales. When considered at the representative elementary volume (REV), Darcy's law is often considered to describe the bulk flow behavior through a variety of geological settings. Adapted from Pankow & Cherry (1996) and Parker *et al*. (2012).

through fractures in consolidated rock, the Forchheimer equation or the Cubic Law may provide a better description of groundwater flow (Forchheimer, 1901; Witherspoon *et al*., 1980, Chin *et al*., 2009). Although when considering groundwater flow at scales typically associated with practical applications, these dynamics often average out across what is sometimes referred to as a 'representative elementary volume' (Fig. 4; Bear, 1972; Freeze & Cherry, 1979; Anderson *et al*., 2015), thereby allowing Darcy's Law to describe the bulk-flow behavior despite underlying complexities. For the purposes and methods used in this thesis, groundwater flow is considered through the framework of Darcy's Law.

In general terms, Darcy's Law is often expressed as:

$$Q = -KA\frac{dh}{dl} \qquad (eq.1)$$

where Q is the volumetric flow rate (L^3/T), K is the hydraulic conductivity (L/T) of the porous material through which the fluid flows, A is the cross-sectional area (L^2) through which the fluid is flowing, and dh/dl is the hydraulic gradient (unitless) between two points where measurements are taken. The hydraulic gradient is sometimes denoted by i, but in the groundwater modelling literature it is more suitably referred to as $grad\ h$, as this relates to the dependent variable hydraulic head (h; L), which numerical models aim to solve for. For consistency with the topic of this thesis, and to avoid confusion with units and indices in later equations and expressions, $grad\ h$ will be used to denote hydraulic gradient. The negative sign indicate that flow occurs from high to low potential energy. Specific discharge (L/T), denoted as q can be written as:

$$q = -K\ grad\ h \qquad (eq.2)$$

In 3-dimensional space, the components of specific discharge in vector form through a representative elementary volume can be expressed as:

$$q = q_x i_x + q_y i_y + q_z i_z \qquad (eq.3)$$

where i_x, i_y, and i_z are unit vectors oriented along the x, y, and z axes. Expressed using partial derivatives, specific discharge contribute to the water balance equation as follows:

$$\frac{\partial q_x}{\partial x} + \frac{\partial q_y}{\partial y} + \frac{\partial q_z}{\partial z} - Q'_s = -S_S\frac{\partial h}{\partial t} \qquad (eq.4)$$

where Q'_s represents the volumetric flow rate (L^3/T) from sources and sinks. Specific storage, denoted S_S (unitless), is defined as the volume of water released from or absorbed into storage per unit change in h over time (t; T) per unit volume of aquifer. The components of q along the x, y, and z axes, governed by hydraulic conductivity, can be expressed as:

$$q_x = -K_x\frac{\partial h}{\partial x} \qquad (eq.5)$$

$$q_y = -K_y\frac{\partial h}{\partial y} \qquad (eq.6)$$

$$q_z = -K_z\frac{\partial h}{\partial z} \qquad (eq.7)$$

where K_x, K_y, and K_z represent the principal components of the tensor K and the derivatives $\partial h/\partial x$, $\partial h/\partial y$, and $\partial h/\partial z$ correspond to the directional components of the vector $grad\ h$. The partial differential equation (PDE) for 3-dimensional transient groundwater flow through anisotropic and heterogeneous media is obtained by substituting Equation 5 into Equation 4 as such:

$$\frac{\partial}{\partial x}\left(K_x \frac{\partial h}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_y \frac{\partial h}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_z \frac{\partial h}{\partial z}\right) = S_S \frac{\partial h}{\partial t} - Q'_s \qquad (eq. 8)$$

In this equation, K_x, K_y, K_z, S_S, and Q'_s are parameters, h is the dependent variable, and x, y, z and t denote the independent variables. For more in-depth derivation of the equations outlined above, the reader is referred to Fetter (2001) and Andersson *et al.* (2015) and references therein.

3.2.1 Advection, diffusion and dispersion

In certain situations, such as when delineating well-head protection areas, or assessing the transport and fate of solutes, calculating transport velocities along with the effects of diffusion and dispersion is beneficial. By extending the concept of specific discharge (q; see Equation 2) to include kinematic porosity, the average linear velocity (v) can be calculated:

$$v = -\frac{K}{\theta} grad\ h \qquad (eq. 9)$$

where v is the average linear velocity (L/T), and θ is the kinematic porosity (unitless), i.e. the portion of the total volume that is occupied by interconnected pore spaces through which groundwater can flow. However, Equation 7 only addresses advective flow within a groundwater system. The advection-dispersion equation (Ogata & Banks, 1961; Freeze & Cherry, 1979) includes the effect of dispersion for non-reactive solutes:

$$\frac{\partial C}{\partial t} = D_x \frac{\partial^2 C}{\partial x^2} - v \frac{\partial C}{\partial x} \qquad (eq. 10)$$

where C represents the concentration of a solute (M/L^3), and D_x is the dispersion coefficient (L^2/T) that accounts for the combined effects of molecular diffusion and mechanical dispersion in the x-direction. When extended to include chemical reactions and transport in 3-dimensional space, the PDE for transport of solutes in a porous, anisotropic, heterogeneous, transient groundwater flow system can be expressed as:

$$\frac{\partial(\theta C)}{\partial t} = \frac{\partial}{\partial x}\left(\theta D_x \frac{\partial C}{\partial x}\right) + \frac{\partial}{\partial y}\left(\theta D_y \frac{\partial C}{\partial y}\right) + \frac{\partial}{\partial z}\left(\theta D_z \frac{\partial C}{\partial z}\right) - \frac{\partial}{\partial x}(\theta v_x C_s) - \frac{\partial}{\partial y}(\theta v_y C_s) - \frac{\partial}{\partial z}(\theta v_z C_s) + q_s C_s + \sum R_n \qquad (eq. 11)$$

where C_s is the concentration of the source or sink flux (M/L^3), q_s denotes the rate of volumetric flow per aquifer volume (T^{-1}), indicating fluid sources (as positive values) and fluid sinks (as negative values), and $\sum R_n$ is the sum of reaction terms, including the effects of chemical or biological reactions affecting the solute concentration. When expressed using tensor notation, Equation 9, also referred to as the advection-dispersion-reaction equation, can be reformulated as described by Zheng & Wang (1999):

$$\frac{\partial(\theta C)}{\partial t} = \frac{\partial}{\partial x_i}\left(\theta D_{ij} \frac{\partial C}{\partial x_j}\right) - \frac{\partial}{\partial x_i}(\theta v_i C) + q_s C_s + \sum R_n \qquad (eq. 12)$$

The sum of reaction terms may be further expanded upon to consider both sorption and first-order rate reactions as follows:

$$\sum R_n = -\rho_b \frac{\partial \overline{C}}{\partial t} - \lambda_1 \theta C - \lambda_2 \rho_b \overline{C} \qquad (eq. 13)$$

where ρ_b represent the bulk density (M/L^3) of the geologic substrate, $\overline{C}$ is the adsorbed solute concentration on geologic particles (M/M^{-1}), and λ_1 and λ_2 is the first-order reaction rate for the dissolved phase (T^{-1}) and sorbed phase (solid; T^{-1}) respectively. For a complete derivation of Equations 8 to 11, the reader is referred to Ogata & Banks (1961), Konikow & Grove (1977), and Zheng & Wang (1999).

3.3 Hydrogeological characterization and parameter estimation

Geological characterization is a broad topic that seeks to interpret and describe the various facets of geological materials and their configurations over one or multiple scales. This characterization can include descriptions of material properties, such as mineralogy, geochemical composition and structural features, or it can cover descriptions of geological processes, such as formation, deformation, erosion and transportation. Characteristics of sedimentary geology are often described in terms of depositional features and stratigraphy, including the types of sediments deposited and the environment they were deposited in (sedimentary facies), bedding thickness and morphology, and variations in grain size and grading, amongst others. Hydrogeological characterization aims to describe the movement of groundwater and solutes within geological materials, focusing on aspects such as the properties of aquifers and aquitards. It often involves identifying units with similar hydrogeological properties, sometimes referred to as 'hydrofacies' (e.g., Meyer *et al*., 2014; Bayer *et al*., 2015). The disposition and spatial variation of these properties tie back to the broader concepts of geological characterization, as these fundamental characteristics control the settings and distribution across different scales, emphasizing the importance of adopting a broad perspective even if the site of interest is small.

In practice, hydrogeological characterization often aims to estimate values of hydrogeological parameters, including hydraulic conductivity (K), specific yield (S_y), specific storage (S_S), amongst others, some of which are detailed in equations 1 to 13. These estimations typically require measurements of either groundwater or the geological materials involved and are often performed at multiple locations within a site to achieve spatial coverage and assess variability. The measurements can be used in empirical, analytical or numerical models to estimate parameter values. Empirical models, for example, include equations for estimating K from the grain size distributions of geological materials (e.g., Hazen, 1892, 1911; Wang *et al*., 2017). Analytical models are widely used to estimate hydrogeological parameters using groundwater measurements collected under various stresses imposed on the hydrogeological system. Pumping tests are often considered the gold standard among these methods, with well-known analytical models that include equations for estimating parameters based on transient data from confined aquifers (e.g., Theis, 1935; Cooper & Jacob, 1946; Moench, 1997), unconfined aquifers (e.g., Boulton, 1954, 1955; Neuman, 1972), and leaky, multi-aquifer settings (e.g., Hantush & Jacob, 1955; Neuman & Witherspoon, 1972). These methods typically operate under a range of idealized assumptions about aquifers, such as infinite extent, homogeneity and isotropy, and depend on hydraulic head measurements, specifically the drawdown and recovery of groundwater during pumping, in monitoring wells spaced around a pumping well. By contrast, the slug test provides a method for analytically estimating parameters without the need for pumping. During this test, a pressure transducer may be lowered into a monitoring well below the groundwater surface, where it records changes in pressure over time. A 'slug', typically a cylindrical metal object, is then lowered into the well, raising the water level. The transducer records the recovery of the water level to equilibrium twice: first when the slug is lowered into the well ('falling head slug test'), and again when it is removed ('rising head slug test') from the well (Fig. 5). A number of analytical models have been developed for the estimation of hydrogeological parameters using slug tests, taking into consideration different aquifer settings and well configurations (e.g., Hvorslev, 1951; Cooper *et al*., 1967; Bouwer & Rice, 1976). Slug tests can be particularly useful in or near contaminated sites, as they allow an estimation of parameters without the risk of mobilizing contaminants.

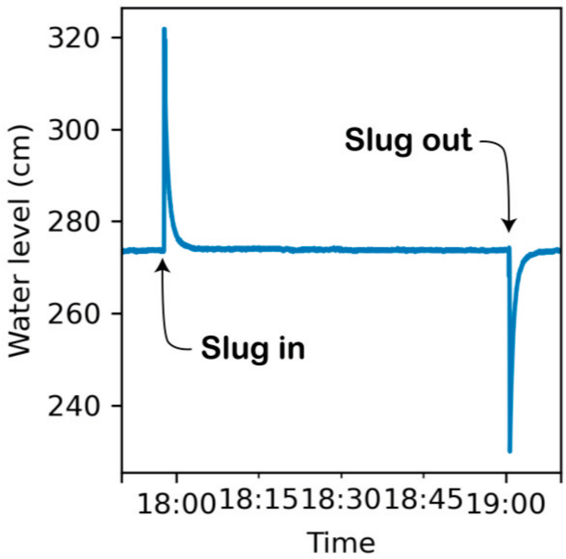

Figure 5. Hydraulic head data sampled at high temporal resolution using a pressure transducer in a monitoring well. The data display the moment a metal slug is lowered into the well, causing an instantaneous rise in hydraulic head, followed by a rapid recovery to equilibrium (falling head). Approximately an hour later, the metal slug is removed from the well, causing a reverse reaction (risning head). These two events allow hydrogeological parameters to be estimated.

Geophysical methods are increasingly important in hydrogeological characterization. Geophysical approaches may involve measuring temperature, electrical resistivity or conductivity and induced polarization, and utilizing techniques such as ground-penetrating radar, transient electromagnetic surveying, magnetometry, seismic and gravimetric surveying (Everett, 2013). Although these methods do not directly provide hydrogeological parameters, information about these parameters can be indirectly inferred. For example, the electrical resistivity of clay-rich sediments, which are typically associated with low permeability, is generally lower compared to that of highly permeable, well-sorted sands and gravels (Samouëlian *et al*., 2005). In settings where interactions between groundwater and surface water play a role, fiber-optic temperature sensing can reveal locations of exchange fluxes (Briggs *et al*., 2012), providing insights into parameters related to the streambed and underlying geology. Geophysical methods can be particularly beneficial for mapping structural features that may be concealed beneath sediments and topsoil. However, given the indirect nature of geophysical responses to subsurface materials, interpretations strongly benefit from supplementary direct observations, such as drill cores and other types of direct sampling, including measurements of hydraulic head or groundwater chemistry, making these approaches complementary.

Another emerging area, specifically in terms of fine-scale site characterization, is the use of methods that rely on direct-push probing. These methods are particularly useful in shallow, unconsolidated settings, where the probe can continuously provide measurements as it is driven through the underground by applied force. A probe can be fitted with multiple sensors, including those for geophysical measurements such as electrical conductivity (Schulmeister *et al*., 2003) or sensors that may provide more direct measurements of hydraulic conductivity, such as the cone penetrometer (CPT; Gribb *et al*., 1998) or the hydraulic profiling tool (HPT; McCall & Christy, 2010). These latter methods rely on injecting small amounts of water into the soil, either under constant pressure while monitoring the volume of injected water (CPT) or under a constant flow rate while monitoring the pressure required to inject water (HPT). Hydraulic conductivity may then be estimated using models elaborated on by Gribb *et al*. (1998) and McCall & Christy (2010), respectively, and further refined in subsequent studies. Over the past two decades, direct-push probing has been widely applied, particularly at contaminated sites, as a method to rapidly obtain high-resolution, multi-point data of various types.

Characterization using numerical methods, particularly inverse methods, is elaborated upon in greater detail in Section 3.5. However, other significant approaches using geostatistical characterization of underground heterogeneity have been developed over the years and warrant mention. These methods usually depend on parameters previously estimated using empirical or analytical methods, or categorical descriptions based on geological interpretation. Examples include kriging interpolation, multi-point statistics (MPS) and transition probability geostatistics (TPG). Kriging is commonly applied as a deterministic method for interpolating parameters within a model domain, using semivariograms to model the spatial correlation between pairwise points present in the data (Sagar *et al*., 2018). By contrast, MPS is employed as a stochastic method that utilizes configurations of three or more points to capture complex spatial heterogeneity, for example sediment deposited in meandering patterns, thereby overcoming the Gaussian assumptions inherent in kriging interpolation (Tahmasebi, 2018). This approach, which typically requires a training image constructed using object- or process-based methods (e.g., Holden *et al*., 1998; Bryant & Blunt, 1992), generates multiple, equally-probable realizations of underground heterogeneity. Likewise, TPG may also generate stochastic representation of underground heterogeneity, but uses an alternative approach which relies on analyzing transition probabilities (Carle & Fogg 1996). With this approach, the spatial distribution of categorical variables, such as various hydrofacies, are modeled using Markov chains (e.g., Lee *et al*., 2007), producing an ensemble of equally-probable realizations that capture the variability of subsurface properties. These stochastic methods can provide useful starting points in terms of assessing the variance of a groundwater model prediction prior to its calibration against measured data.

3.4 Simulation of groundwater flow and transport

As a note, this subchapter is explicitly named 'Simulation of groundwater flow', rather than, for example, 'Groundwater modelling'. This is a conscious decision to clarify the distinction between the two concepts, which has been identified as a point of uncertainty, particularly in the Swedish industry. As discussed in Paper 1, and as approached in this thesis, the concept of groundwater modelling consists of multiple components, of which the simulation is an important (but not the only) part of a robust modelling workflow. Other important components, such as data assimilation and uncertainty quantification, are elaborated upon in the subsequent section.

Simulation enables quantitative analysis of groundwater flow and ancillary processes such as solute transport within a defined area using mathematical models that are solved numerically (hence the term 'numerical model'). The application of numerical methods in hydrogeology was first introduced by Stallman (1956), who recognized a need to move beyond analytical methods for solving groundwater-related issues. This need was especially evident at regional scales, where the idealization of aquifers as homogeneous systems of infinite extent, an assumption inherent in many analytical models, was particularly unrealistic. Fayers & Sheldon (1962) were among the first to utilize a digital computer to iteratively solve the steady-state groundwater flow PDE using the finite difference method. Their model utilized a combination of Dirichlet (specified head) and Neumann (specified flow) boundary conditions with a curvilinear, layered, three-dimensional mesh based on geological interpretation. This emerging subject was further pioneered by Freeze (1967), who highlighted the impact of heterogeneity on steady state simulation, and by Pinder & Bredehoeft (1968) who developed a program for solving transient groundwater flow in confined aquifers. In the following years, the advancement and refinement of these methodologies was largely led by the U.S. Geological Survey (USGS; e.g., Bredehoeft & Young, 1970; Trescott, 1975; Winter, 1978; Konikow & Bredehoeft, 1978), ultimately leading to the development of the famous MODFLOW code during

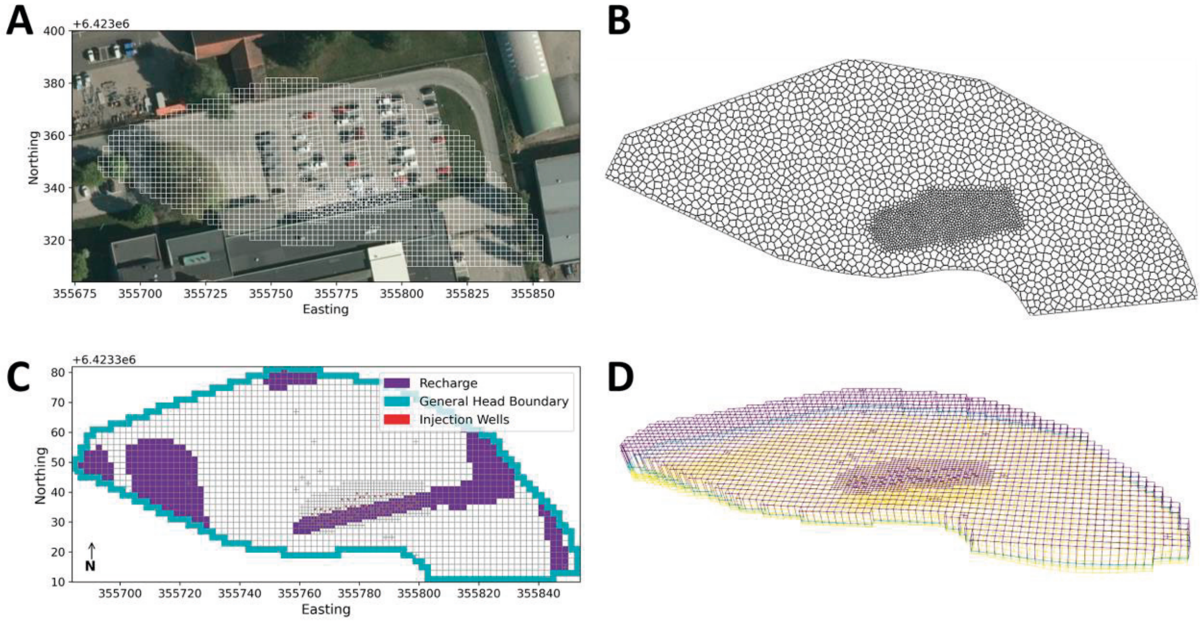

Figure 6. Variation in model grid design and boundary condition placement. A) and B) display a quadtree grid and a Voronoi grid, respectively, both featuring local refinement around monitoring wells and injection points. C) illustrates the different types and locations of boundary conditions such as recharge, injection wells and boundaries of the model domain, typically encountered and arranged according to the local setting. D) shows a 3-dimensional view of the model grid, with each layer represented by a unique color. The coordinate system is SWEREF99TM.

the 1980s (McDonald & Harbaugh 1988; 2003). To this day, MODFLOW continues to be supported by the USGS (Langevin *et al*., 2017), and, although other groundwater flow simulators have been written over the years, it is still considered an industry-standard software. Today, it is incorporated into many commercial graphical user interfaces (GUIs), enabling hydrogeologists to simulate groundwater flow without requiring prior experience in programming.

Numerical simulation software solves extensions of Equation 6 for groundwater flow, Equation 7 for flow velocities and particle tracking, and Equation 10 for solute transport and reaction, across one to three dimensions, utilizing either the finite-difference method (e.g., MODFLOW) or the finite-element method (e.g., HYDRUS, FEFLOW, and FEMWATER). Although these latter methods differ in their approach for approximating values of the dependent variable, both can provide similar results (Key & Krieg, 1973; Anderson *et al*., 2015). Historically, the finite-element method has been favored by some for its capability to represent complex geometries. However, recent implementations of the control volume finite-difference method in MODFLOW have enabled flexible meshing capabilities comparable to those available in finite-element programs (Fig. 6; Panday *et al*., 2013; Langevin *et al*., 2017), facilitating simulation over multiple spatial scales within the same model domain.

During numerical solution of the groundwater flow equation, the dependent variable (hydraulic head) is approximated at the nodes within a model's mesh. This approximation process involves iterative calculations using a solver, which continues until the solution meets a predefined error tolerance specified by the user. Boundary conditions control how the model solution is influenced by interaction with ancillary processes of the hydrological cycle, including recharge, groundwater-surface water exchange, interaction and exchange at the model's edges, and stresses induced by management actions such as pumping. Temporal discretization allows simulations to be conducted under both steady-state and transient conditions, permitting the user to define the temporal resolution to model dynamic changes over time, tailored to the objectives of the study.

Several key factors are central to the usability of groundwater simulation in its decision-support role. These include the quality of input data, the methods used for estimating parameters and assimilating data (Doherty & Moore, 2020), how uncertainties in geological interpretation are propagated through the model (e.g., Enemark *et al*., 2024), and the quantification of predictive uncertainty (Caers, 2011). These concepts are elaborated on in the following sections.

3.5 Data assimilation and uncertainty quantification

This section begins by continuing with the topic of parameter estimation, now within the context of inversion modelling (Fig. 7) and under the broader framework of 'data assimilation'. Data assimilation encompasses methods that enhance the predictability of numerical models through assimilating observations of system state (Fletcher, 2017), for example, measurements of hydraulic head or the concentration of a solute. By iteratively adjusting (estimating) model parameters, the difference between observed and simulated data, often referred to as

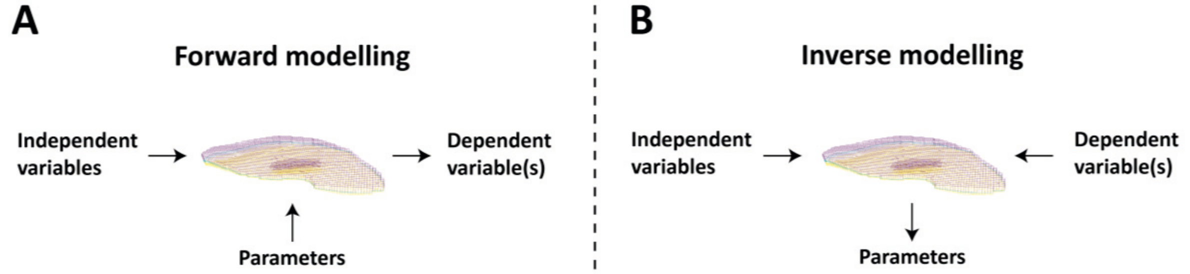

Figure 7. The flow of information under A) forward modeling, and B) inversion modeling. Data, which are more easily measured in the field and correspond to the dependent variable(s), are assimilated through inverse modeling to solve for parameters. Predictive uncertainty can then be explored through forward modelling by employing all parameter variations that exist within the constraints of calibration.

'residuals' or 'error', can be reduced (Fig. 8). In the context of numerical modelling, this process is often referred to as 'calibration' or 'history matching'. To estimate parameters effectively, an optimization algorithm is typically employed. This algorithm seeks to minimize an objective function, which is related to these residuals. Common objective functions in the field of machine learning include Mean Squared Error (MSE), Mean Absolute Error (MAE), and Mean Absolute Percentage Error (MAPE). In the context of groundwater modelling, a commonly-used objective function is Weighted Mean Squared Error (WMSE; often referred to as the Sum of Square Weighted Residuals in groundwater literature), which can be expressed as:

$$\Phi = \sum (w_i r_i)^2 \qquad (eq. 14)$$

where w_i and r_i represent the weight and residual of the i'th observation respectively. This objective function is particularly useful in groundwater modelling because it allows the modeller to assign higher weights to more trustworthy or important observations, and vice versa, thereby imposing subjectivity into the workflow that is both desirable and necessary (Fienen, 2013; Kalantari *et al*., 2015). For example, a modeller may implement strategies that assign greater importance to specific types of observations, or those recorded at particular locations, dates, or seasons, by increasing their weights accordingly. Consequently, the value of the objective function reflects the weighting strategy employed, allowing the optimization algorithm to estimate the optimal set of parameters that minimize this value, as shown in Equation 14. The Gauss-Levenberg-Marquardt algorithm (GLM; Levenberg, 1944; Marquardt, 1963) and its variations have been developed to solve nonlinear least squares problems and implemented in industry standard calibration codes (e.g., Doherty *et al*., 1994; Poeter & Hill, 1999; White *et al*., 2020) and have served as the foundational algorithm in groundwater modelling for many years. This algorithm iteratively searches the surface of the objective function for its minimum value, as visualized in a simple, synthetic, two-dimensional (two-parameter) problem by Hugman *et al*. (2022; Fig. 9). During each iteration, as implemented in PEST (Doherty, 2015) using a slightly modified notation, model parameters are estimated according to GLM in the following equation:

$$\Delta_\theta = (J^T Q J + \lambda I)^{-1} J^T Q r \qquad (eq. 15)$$

where Δ_θ represents the change in the parameter vector, J is the Jacobian matrix of partial derivatives of the residuals with respect to the parameters, Q is the weight matrix, λ is the damping factor (also referred to as the Marquardt lambda) which controls the step size between iterations, I is the identity matrix, and r is the vector of residuals. As shown (Fig. 9), the shape of the objective function surface can vary depending on the model configuration, as well as the number and types of observations used. Although the objective of the GLM is to identify the set of parameters that represent the global minima of the objective function, this algorithm may become stuck in local minima, which can lead to the erroneous reporting of an unoptimized solution as an optimized one. Additionally, many cases requiring a higher degree of model complexity, such as those involving real sites, may represent ill-posed inverse problems. This implies the possibility of multiple solutions (or parameter combinations), that can calibrate a model equally well, a phenomenon also known as parameter non-uniqueness. This phenomenon was famously demonstrated in a paper by Freyberg (1988), in which groups of students undertook manual (trial-and-error) calibration of a groundwater model, showing that a well-calibrated model did not necessarily lead to good predictions. To obtain a unique solution in an ill-posed setting, different regularization methods can be applied. For example, the dimensionality of the inverse problem can be reduced using singular value decomposition (SVD) to identify superparameters. The inverse problem can be further regularized by imposing penalties to the objective function value on solutions as they deviate from prior parameter values. This approach, known as Tikhonov regularization, is particularly useful in groundwater modelling as it allows the modeller to incorporate expert knowledge into the calibration process. By gauging the extent to which certain parameters may deviate from their initial values, more trusted parameters are kept closer

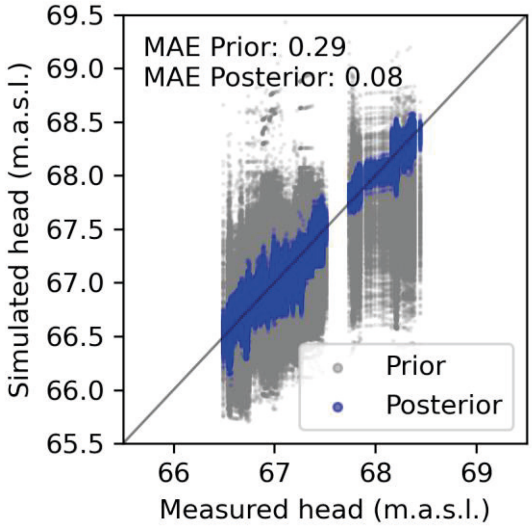

Figure 8. Reduction of error in simulated hydraulic head compared to measured (observed) head before calibration (prior) and after calibration (posterior). For improved relatability to the dependent variable, in this case hydraulic head, this illustration shows Mean Absolute Error (MAE) instead of Weighted Mean Squared Error (WMSE), which is the objective function that PEST typically seeks to minimize.

to their original values, while less certain ones are allowed greater variability.

Although great efforts can be made to reduce uncertainties in observations, for example by using precise and sophisticated measurement equipment, uncertainties in model parameters and model structure can still be substantial, even with high-quality observations. These uncertainties, pertaining to both observations and the model and its parameters, propagate through to the predictions the model is designed to make. To serve as an effective and informative decision-making tool, it is fundamental that uncertainties in predictions are not only reduced through calibration but also quantified. In essence, decision-support modelling undertaken using inversion codes, such as PEST, implement Bayes' theorem for this purpose (Ferré, 2020). Bayes' theorem is often expressed as:

$$P(a|b) = \frac{P(b|a)P(a)}{P(b)} \qquad (eq. 16)$$

where $P(a|b)$ is the conditional probability that event a will occur given that b is true, $P(b|a)$ is the conditional probability that event b will occur given that a is true, and $P(a)$ and $P(b)$ are the probabilities of a and b occurring irrespective of each other. By letting vector k denote the model parameters, and vector h denote historical measurements of system state (observations) including measurement noise, Equation 16 can be written as described by Doherty (2015):

$$f(k|h) = \frac{f(h|k)f(k)}{f(h)} \qquad (eq. 17)$$

where $f(k|h)$ is the posterior probability density function (PDF) of parameter vector k given observation vector h. As parameters are updated during history-matching (calibration), the PDF transitions from prior to posterior, reflecting updated knowledge as data is assimilated by the model. Predictive uncertainty may be explored by sampling both the prior PDF $f(k)$, and the posterior PDF $f(k|h)$. Furthermore, the differences between these distributions reflect the reduction in uncertainty achieved during history-matching (Fig. 10).

While there are numerous ways to formulate the prior PDF, $f(k)$, ranging from simple random sampling to more sophisticated geostatistical approaches like MPS and TPG as outlined in Section 3.3, sampling the posterior requires the application of uncertainty analysis methods on a model that has undergone history matching. These methods include rejection sampling, Markov-chain Monte Carlo, calibration-constrained Monte Carlo, and ensemble methods. In the context of groundwater modelling, which is typically associated with long model run

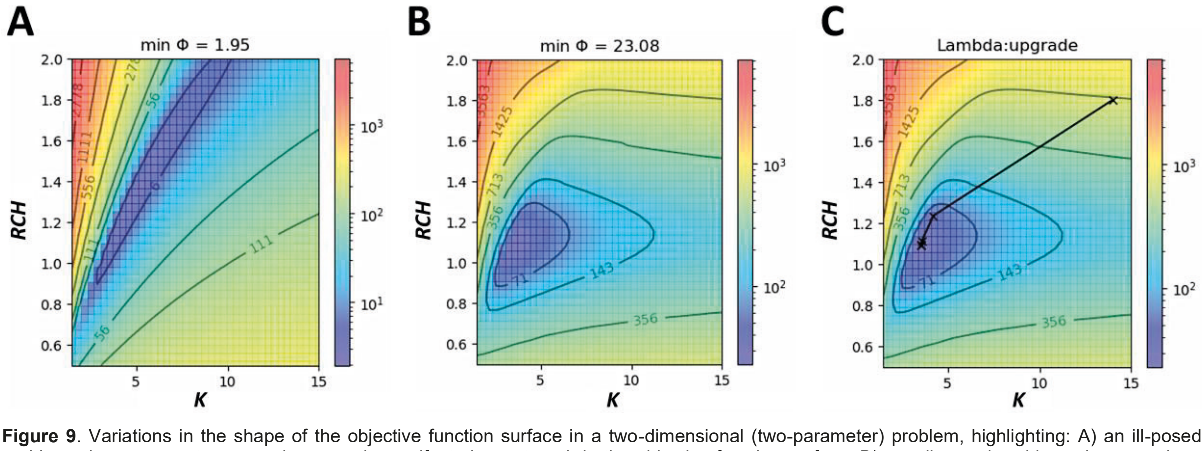

Figure 9. Variations in the shape of the objective function surface in a two-dimensional (two-parameter) problem, highlighting: A) an ill-posed problem where parameter non-uniqueness is manifested as a trough in the objective function surface; B) a well-posed problem where a unique solution can be identified, manifested as a bowl in the objective function surface; and C) adaptive descent along the objective function surface over three iterations as parameter values for recharge (*RCH*) and hydraulic conductivity (*K*) are adjusted by PEST. Adapted from Hugman *et al*. (2022).

times, rejection sampling proves inefficient and is thus rarely used. Markov-chain Monte Carlo methods (e.g., Vrugt & Ter Braak, 2011) provide a more efficient and robust alternative to rejection sampling, although efficiency deteriorates as the number of parameters increases. Calibration-constrained Monte Carlo allows for the exploration of predictive uncertainty by utilizing a combination of different parameter sets that fit the measured data within a specified threshold. This method assumes that the model has been calibrated first, allowing for the construction of a covariance matrix of parameter error with respect to model predictions (Doherty, 2015). The most common variation of this method, called the null-space Monte Carlo, efficiently handle highly parameterized models through parallelization of model runs, and is implemented in several well-known commercial modelling codes, such as GMS and Visual MODFLOW Flex.

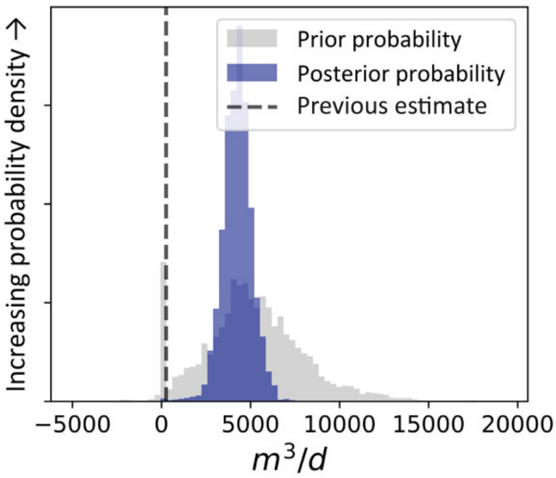

Figure 10. The prior and posterior probabilities of a prediction pertaining to surface water-groundwater exchange flux at a contaminated site, calculated using the IES with 500 realizations. The dashed line marks the calculated exchange flux from a previous study that relied on a deterministic approach; a single realization that underwent manual calibration (trial-and-error). Adapted from Paper II, (Benavides Höglund *et al.* 2023) in this thesis.

Ensemble methods, particularly the iterative ensemble smoother (IES; Chen & Oliver, 2013; White, 2018), have gained significant popularity in recent years for their ability to assimilate large datasets and manage very high parameter dimensionality without increased run times. This is because the number of parameters is detached from the number of model runs required for history matching. Additionally, the IES can accommodate simultaneous predictive uncertainty analysis as part of the inversion process. The parameter estimation algorithm is an ensemble variation of GLM, in which vectors of parameters and observations are replaced by matrices, thereby representing multiple realizations (an ensemble) of parameters and observations. As implemented in PEST++ (White *et al.*, 2020), the IES variation of Equation 15 is modified into:

$$\Delta_\Theta = -(J^T \Sigma_E^{-1} J + \lambda \Sigma_\Theta^{-1})^{-1} \Sigma_\Theta^{-1} (\Theta_0 - \Theta) + J^T \Sigma_E^{-1} (D_{sim} - D_{obs}) \qquad (eq. 18)$$

where Δ_Θ represents the change in the parameter ensemble, Σ_E^{-1} is the inverse of observation noise covariance matrix, Σ_Θ^{-1} is the inverse of the prior parameter covariance matrix, Θ_0 is the prior parameter ensemble, Θ is the current parameter ensemble, and D_{sim} is an ensemble of simulated outputs corresponding to D_{obs}, which is an ensemble of observations complemented with realizations of added measurement noise. Note that the matrix Σ_E^{-1} corresponds to the matrix Q, and that the matrix $(D_{sim} - D_{obs})$ is the ensemble form of vector r in in Equation 15, respectively. Because the IES adjusts ensembles of parameters, as opposed to the GLM which adjusts individual parameters, the number of model runs needed to populate the Jacobian matrix is determined by the number of ensemble members (realizations), rather than by the number of adjustable parameters. This liberates the modeller to increase the number of parameters without negatively impacting the total run time, thereby facilitating parameterization of complex geology (Hunt *et al.*, 2021). Using ensemble methods, the results of model predictions are assessed through all members of the ensemble and are therefore inherently probabilistic. This makes them compatible with the further integration of other risk models, such as economic risk.

3.6 Value of information

Characterizing the underground in sufficient detail for a given task or prediction is often associated with considerable cost, both in terms of time spent in the field, and money spent on equipment and analyses. Additionally, fieldwork is typically divided into various phases, including initial investigations followed by activities such as drilling, coring, sampling, pumping, treatment, or implementation of other groundwater affecting actions. It is also common to implement a monitoring program to continuously track the environmental impacts and effectiveness of each of these actions. These phases, or parts of them, may be repeated multiple times as time progresses, situations evolve and new information becomes available.

Using techniques that allow decision-makers to explore the value of data, often referred to as 'data worth' in the groundwater literature, can significantly enhance the effectiveness of data acquisition efforts (Kikuchi, 2017). Data worth is evaluated using numerical models to assess how data reduces the uncertainty of critical management predictions, such as forecasts of groundwater levels or contaminant pathways. Traditionally, this approach relies on linear analysis in which the Jacobian matrix is filled by evaluating the model once for each parameter (White *et al*., 2020), estimating the sensitivity of observations to small changes in parameter values (parameter perturbation). It also requires that a sensitivity vector with respect to the prediction, as well as two covariance matrices, be calculated, one expressing expected parameter covariance and another measurement noise (Fienen *et al*., 2010; Doherty, 2015). As demonstrated by Dausman *et al*. (2010), the posterior uncertainty (variance) of a prediction s can be calculated as:

$$\sigma_s^2 = y^T[X^T C^{-1}(\varepsilon)X + C^{-1}(p)]^{-1}y \quad (eq. 19)$$

where the vector y represent the sensitivity of a prediction to model parameters, X is the Jacobian matrix of sensitivities under calibration conditions, $C^{-1}(\varepsilon)$ is the inverse of the measurement noise covariance matrix, and $C^{-1}(p)$ is the inverse of the prior parameter uncertainty covariance matrix. An important implication of Equation 19 is that it does not rely on the parameter values or model outputs themselves, but solely on their sensitivities. Consequently, not only can the worth of existing data be estimated, but through the addition of synthetic observations and a subsequent recalculation of the Jacobian matrix, the worth of future potential data can also be estimated (e.g., Gosses & Wöhling, 2021). Typically, the worth of data is explored in two ways: By measuring the increase in predictive uncertainty when existing observations or groups of observations are removed (effectively setting their weight to zero) or by measuring the decrease in predictive uncertainty when new observations are added. The worth of different types of data, including their value related to geographic location and time, can be assessed. In this manner, data acquisition campaigns can be optimized by sequentially identifying the next most important potential observation through iterative addition of synthetic observations (e.g., White *et al*., 2016; Partington *et al*., 2020).

As mentioned, the manner in which the Jacobian matrix is populated differs between the IES and GLM algorithms. With the GLM, sensitivities are calculated using parameter perturbation, which implies causality between the parameter changes and the variations in model outputs (White *et al*., 2020). By contrast, the IES approximates sensitivities through empirical cross-covariances between parameters and observations. Concerns have been raised regarding this difference and their implications for the suitability of the IES-derived Jacobian matrix in data worth analyses (e.g., White *et al*., 2020). However, two recent studies (He *et al*., 2018; Delottier *et al*., 2023) have benchmarked the difference between linear and nonlinear methods in assessing posterior predictive uncertainty and data worth, finding broad agreement between these approaches. The method presented by He *et al*. (2018), referred to as ensemble variance analysis (EVA), has in a recent software update been implemented in PyEMU, a Python interface for constructing PEST-based workflows (White *et al*., 2016). Unlike linear analysis, which rely on parameter uncertainty covariance matrices (e.g. as shown in Equation 19), EVA utilizes the cross-covariance between predictions and observed data to directly address prediction uncertainty. This approach utilizes ensembles of observed values D_{obs} (realizations of added measurement noise; now denoted d for consistency with He *et al*., 2018) to calculate the expected posterior variance of a prediction (now denoted f, 'forecast', to avoid conflation with expressions in Equation 19):

$$E_d\left(\sigma_{f|d}^2\right) = \sigma_f^2 - \Sigma_{fd}\Sigma_{dd}^{-1}\Sigma_{fd}^T \quad (eq. 20)$$

where $E_d\left(\sigma_{f|d}^2\right)$ is the expected posterior variance of prediction f averaged over all realizations of d, σ_f^2 is the prior predictive variance, Σ_{fd} is the cross-covariance matrix between the prediction f and the data d, and Σ_{dd}^{-1} is the inverse of the covariance matrix for d. In this equation, Σ_{fd} reflects how the uncertainty in f is reduced by the information provided by d. As suggested by He *et al.* (2018) and implemented in PyEMU to provide ease of comparison between different types of observations, Equation 20 can be rearranged into:

$$1 - \frac{E_d\left(\sigma_{f|d}^2\right)}{\sigma_f^2} = \frac{\Sigma_{fd}\Sigma_{dd}^{-1}\Sigma_{fd}^T}{\sigma_f^2} \quad (eq. 21)$$

in which the left-hand side express the predictive uncertainty reduction as a percentage of the prior uncertainty, given data d. In the context of this thesis, Equation 21 is used to quantify the value of data with respect to predictions presented in Paper IV, as well as in unpublished results pertaining to the predictions in Paper II, which are presented in Section 6 and further discussed in Section 7.

4 The study sites

This thesis is based on work conducted in two primary categories. The first category includes field methods such as coring, sampling, and aquifer stress testing, which utilize both manual measurements and measurements recorded using sensitive data logging equipment. The second category encompasses data curation, interpretation, and analysis, as well as numerical methods including simulation, data assimilation, and uncertainty quantification. Fieldwork was conducted at two sites in Sweden (Fig. 11), both contaminated with PCE due to spills that occurred during their previous use as industrial-scale dry-cleaning facilities. This section provides a brief introduction of the two sites; their history, past work, location and geological settings is described in detail in Papers II, III, and IV. The materials and methods used in the gathering of field data, as well as the numerical methods and modelling workflows employed, are presented in the subsequent section.

4.1 The Hagfors aquifer

The decommissioned dry-cleaning facility in Hagfors was formerly used by the Swedish Armed Forces between the 1970s and the 1990s (Nilsen & Jepsen, 2005; SEPA, 2007). The site is located adjacent to residential buildings in three directions and an industrial area to the west. It is situated on highly conductive glaciofluvial sediment, visible in the form of an esker just to the north of the site (Gustafsson, 2017). The glaciofluvial deposits extend in a NE-SW direction and are partially eroded in the SW of the site where a ravine is present. This sediment is overlain by fill material in the area where the facility is located and serves to flatten the topography for nearby structures and a railroad that was formerly present. A creek, Örbäcken, flows through the site and down through aforementioned ravine (Fig. 12). The depth to the groundwater table varies from approximately 14 m beneath the surface where the facility is located, to 0.5 m beneath the surface in the ravine. Historically, this area was used for groundwater abstraction for drinking water purposes due to the favorable hydrogeological setting, and old wells predating the facility are present. The contamination was discovered during an effort to re-investigate the area's potential for use as a backup municipal water supply. It is believed that large amounts of PCE (50 tonnes or more; Nilsen, 2013) have been spilled at the site, with the majority having been disposed of through a shaft in the facility floor. Because a secondary source zone has been located beneath the bank of the creek approximately 150 m south of the facility where a pipe opens, it is believed that, at some point, the method of disposal was changed to dumping in the creek area. In this area, free-phase PCE is still found in the interface between the crystalline bedrock and unconsolidated sediment (Nilsen, 2013; Åkesson, 2019). It is estimated that approximately 130 kg of groundwater-dissolved PCE is discharged into the creek every year (Nilsen, 2013; Larsson, 2020; Paper II). Prior attempts by environmental agencies to remediate the source zone have proven difficult, with numerous campaigns over the years collectively achieving only about 15 percent removal of the estimated total contaminant leaked into the ground. Because the creek, which flows through a residential area, is the primary source of exposure to the contaminant and discharges into a nearby lake, mitigating influx into the creek has been the focus for SGU and associated environmental consultants. For this reason, assimilating pertinent data regarding the dynamics of surface water-groundwater exchange flux is a priority. This subject was the focus in the study of Paper II.

Figure 11. Map of Sweden showing the location of the two field sites, situated in the towns of Hagfors and Alingsås, using the national coordinate system SWEREF99TM.

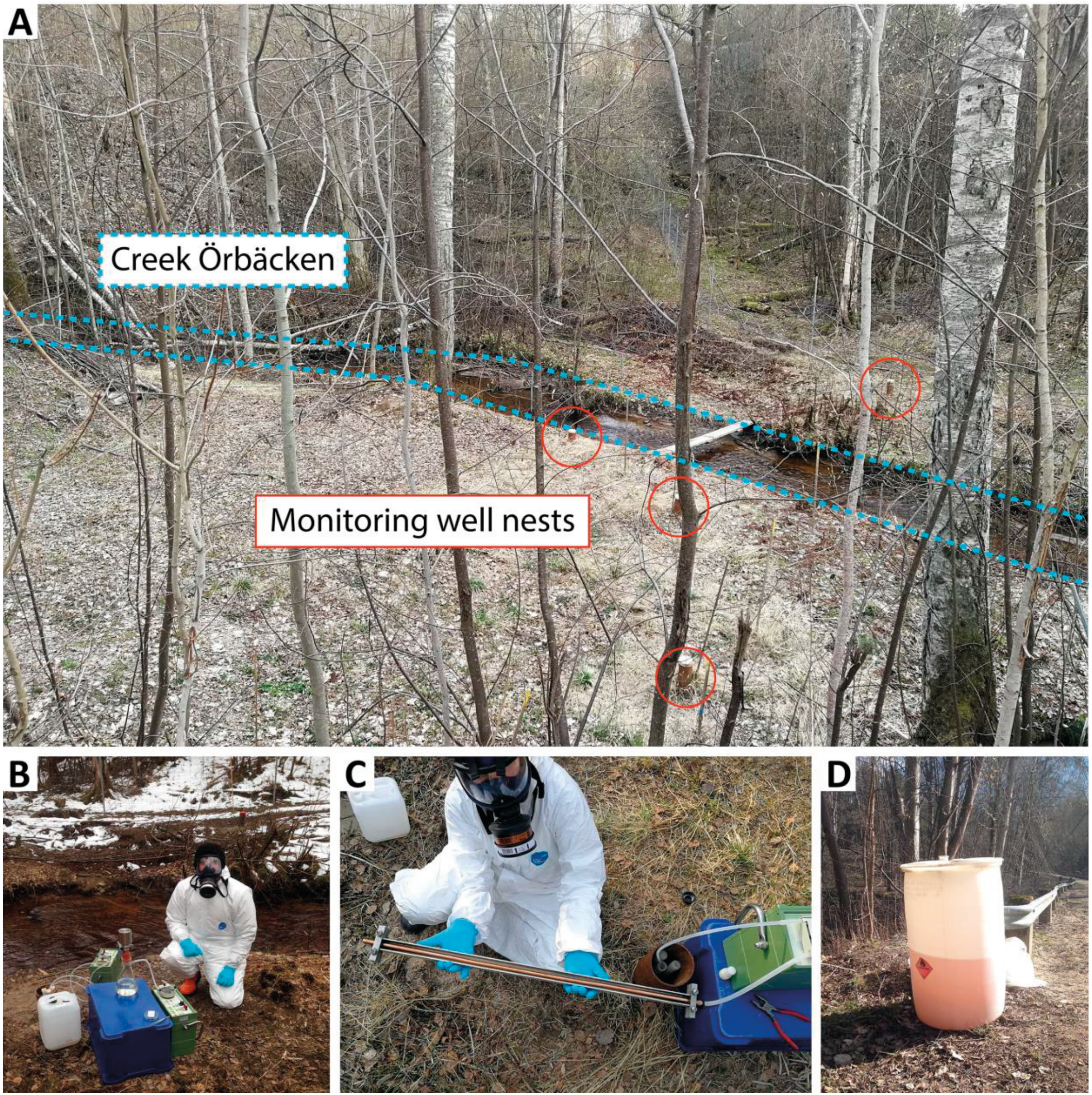

Figure 12. Photographs from the ravine at the Hagfors former laundry site during fieldwork campaigns in April of 2017 and 2019, respectively. A) This photo provides an overview of one of the sampling locations adjacent to creek Örbäcken. Width of creek is approximately 6-8 m. It highlights the location of monitoring well nests (each nest contains up to three monitoring wells, filtered at different depths), from which samples were collected. B) and C) show the use of peristaltic pumps for pumping and sampling. D) displays a high-density polyethylene barrel used for the temporary disposal of contaminated water, which prevents the reintroduction of extracted contamination into the environment before shipment for proper disposal.

4.2 The Alingsås laundry

The Alingsås laundry is an industrial-scale facility currently operating for the administrative region of Västra Götaland, providing laundry services for hospitals in Sweden's second-most populous region. The facility (Fig. 13) has been in operation since the 1960s, but the use of PCE ceased in the early 2000s. During this period, a spill of 200 liters was documented (Cedhagen, 2002); however, the possibility of additional undocumented spills cannot be ruled out. The site is situated on the southern edge of a valley east of the town center, with a surface topography gently dipping towards the NNW. The facility is located in an industrial area, approximately 600 m from the potential recipient, the river Säveån. Outcrops of crystalline bedrock are visible a few meters south of the facility. While in use, the dry-cleaning machines, including a tank used for collecting the spent fluid, were located in the northeastern corner of the facility. This location is identified as the source zone for the PCE contamination at the site. Beneath this part of the facility, the underground consists of silty clay in the uppermost 3 m, followed by approximately 2 m of silty sand and coarse sand. The depth to the bedrock varies from approximately 5 meters in the southeastern part of the study area to about 15 meters where the bedrock dips steeply towards the NNW, in the direction of the valley floor. As a result, the thickness of the sediment increases in this direction

Figure 13. Photographs from the Alingsås laundry site during a fieldwork campaign in October 2020, illustrating A) a sonic drilling rig in operation, and B) the extraction of a drill core. C) displays parts of the outdoor fieldwork laboratory with core sections mounted on a rack for logging and sampling. D) highlights a transmissive fracture in an otherwise tight, clayey silt segment of one of the cores. E) shows the process of sampling in a well-sorted sandy segment within a core, and F) shows a collection of samples gathered for chemical and grain size analysis prior to shipment to the laboratory.

(Branzén, 2016). A parking lot is located outside the facility's northern boundary, beneath which a plume of PCE and its metabolites have been found migrating in a NNW direction. Here, the groundwater table is situated approximately 1.5 meters below the surface. Small amounts of free-phase PCE are likely still present beneath the source zone, but measured concentrations and a strong presence of metabolites suggest that most of the contaminated mass has either dissolved or been adsorbed onto particles of the soil matrix (Forsberg & Davidsson, 2018).

The site underwent an in-situ pilot remediation test during November and December 2017 (Ølund, 2017), during which remediation fluids were injected into the plume beneath the parking lot. The design of the remediation program was based on in-situ characterization, utilizing MIP and HPT probes at multiple locations across the parking lot, undertaken eight months prior to the remediation (Balzarini, 2017). Monitoring of the remediation injections was conducted using a combination of high-frequency transducer sampling and geophysical techniques, as detailed in Paper III and IV. My main contribution to Paper III involves utilizing the high-resolution data from MIP and HPT probes to enhance the interpretation of geophysical results obtained by

DCIP. Further insights into the application and impacts of the rapid rate of injections and the assimilation of the hydraulic response data are discussed extensively in Paper IV.

5 Materials and methods

5.1 Field methods and data collection

Data collection at the study sites involved the application of various methods, including groundwater chemistry sampling and taking hydraulic head measurements in monitoring wells, drill core logging and sampling, and direct push logging. Among these, monitoring wells played a critical role, not only offering insights into the sediment thickness and disposition but also providing calibration data for the numerical models. Most monitoring wells were solitary, 5 cm in diameter, and fully penetrated the unconsolidated sediment. Filter screens were placed at the bottom meter just above the interface between the crystalline bedrock and the sediment, generally ranging between 8 to 20 meters beneath the ground surface at both sites. At the Alingsås site, however, a minority of wells were designed with filter screens at the bottom two meters. At both sites, nests of partially penetrating wells were also installed (e.g. Fig. 12 A), which were filtered at varying depths in the unconsolidated sediments. This configuration provided information on the vertical variability in heads, permeability and groundwater chemistry. Before pumping or any other actions affecting the groundwater were conducted, initial measurements in all monitoring wells were recorded using manual level meters (Fig. 14). Pressure transducers, including the TD-Diver, Micro-Diver, and Campbell Scientific CS456, were used to continuously record high-resolution water level measurements. These instruments recorded changes during applied stresses such as injections and pumping, as well as ambient changes in hydraulic head over weeks and months of monitoring. Before sampling, purging was performed using a peristaltic pump, and water parameters were monitored using a flow cell with sensors for dissolved oxygen, electrical conductivity, pH, oxidation-reduction potential, temperature and total dissolved solids, to ensure sampling of groundwater from the actual formation (Fig. 14). Purged water was disposed of in high-density polyethylene barrels (Fig. 12 D) which was later shipped for destruction to avoid reintroducing contaminants into the ground. Sampling

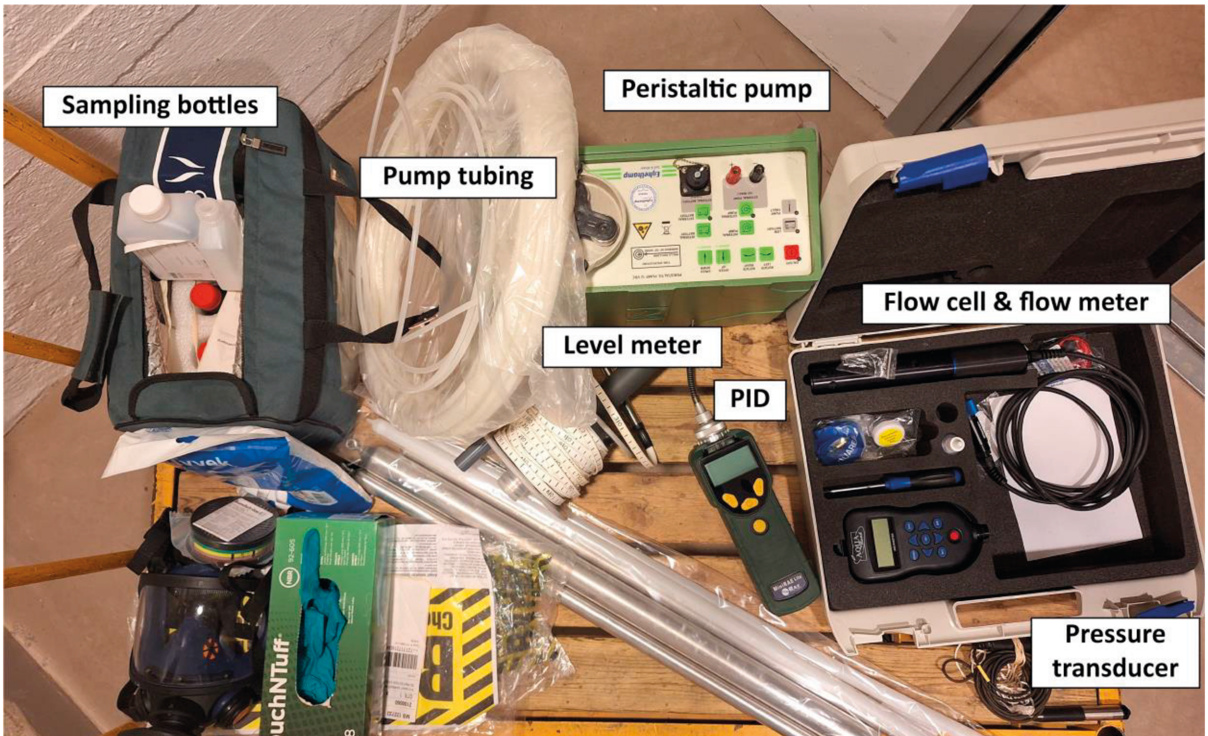

Figure 14. Photograph of equipment frequently used during fieldwork at the two sites.

and testing began once a reasonably steady state in these parameters had been obtained (e.g. 12 B-C). Slug tests were conducted using aluminum cylinders for both falling and rising head tests. Plastic bailers (Fig. 14) were used for rising head tests in wells where the hydraulic head and ground level were too close to perform falling head tests without causing water overflow. Pressure transducers were used to record the pressure response to the slug tests. The pressure data were converted to water-level data using barometric compensation before evaluation following Hvorslev (1951) and Bouwer & Rice (1976) to estimate parameters. More detailed information on the slug tests conducted at the Alingsås site is presented in Björn (2019).

Drill cores at the Alingsås site were collected using sonic drilling (Fig. 13 A-B) during a field campaign in October 2020. This method utilizes high-frequency vibration to penetrate the underground without the need for drilling mud, water, or air to lubricate or cool the drill bit. Such an approach is particularly suitable for environmental applications where preserving the core's details and chemical composition is important for interpretation, sampling, and analysis. Twelve cores ranging between five to twelve meters long were retrieved in segments of approximately 1.5 m each. Upon extraction from the drill pipes, the cores were sealed using cylindrical plastic bags. Presence of volatile organic compounds was examined using a photo-ionization detector (PID) before extracting the cores from their sealing. Once extracted, the core surface was scraped clean using spatulae. Depending on the cohesiveness of the material, the core was then either split or further scraped to reveal details necessary for core logging (Fig. 13 C). Where the PID indicated the presence of volatile organics, sampling was prioritized over detailed logging to mitigate the escape of these compounds. Samples of the core material were collected for both geochemical and grain size analyses (Fig. 13 D-F). These samples, along with groundwater chemistry samples extracted from monitoring wells, were shipped to a third-party, Swedac-accredited laboratory, SYNLAB Sverige AB (formerly ALControl), for analysis. Results from the grain size analyses were used to estimate hydraulic conductivity values using the method of Wang *et al*. (2017). All field work that required contact with contaminated soil and groundwater was conducted using protective gear (Fig. 12 B-C and Fig. 14) designed to resist stains and filter out chlorinated solvents in both liquid and gaseous forms.

During the studied periods, the research project associated with this thesis collaborated with the environmental consultancies Sweco Sverige AB, NIRAS Sweden AB, Tyréns Sverige AB, and WSP Sverige AB. These partners have been involved in various site activities, including installing monitoring wells, performing in-situ characterization using the membrane interface probe (MIP), the HPT, and sampling conventional data such as groundwater chemistry. Data sharing within this collaboration was supervised by the SGU, which holds legal responsibility for site remediation at both sites. Some of the data used in this thesis were sampled as part of this collaboration and have been published in technical reports, which are cited in the papers and manuscripts of this thesis. In addition, the fieldwork and data collection undertaken in this project were partially a joint collaborative effort between parallel Ph.D. projects (Åkesson, 2022; Nivorlis, 2023).

5.2 Data analysis and modelling workflows

The data gathered during fieldwork, combined with data published in technical reports, provided the basis for the development and calibration of the groundwater numerical models at the two study sites. Analytical work, which included data analysis and preprocessing, model design and construction, as well as the analysis of results and construction of figures, was carried out using the Python scripting language (van Rossum & Drake, 1995) through the interactive browser-based programming platform Jupyter Notebook (Fig. 15 A; Kluyver *et al*., 2016). This approach facilitated troubleshooting and interoperability across the various platforms used for different parts of the work, such as the Windows and Linux operating systems. Pandas (McKinney, 2012) and NumPy (Oliphant, 2006) were extensively used for processing and curating data, such as transforming field data into calibration datasets and constructing model temporal discretizations, among other tasks. For GIS-specific tasks, such as sampling elevation data and intersecting model grids, Rasterio, Fiona, and Shapely (Gillies *et al*., 2013; 2016; 2024) were used. GeoPandas (Jordahl *et al*., 2020), in conjunction with Matplotlib (Hunter, 2007), was used for creating maps, while graphs and charts were created using Matplotlib. The remaining figures were created using Adobe Illustrator.

The groundwater models were constructed using MODFLOW6 (MF6; Langevin *et al*., 2017) through the Python library FloPy (Fig. 15 A; Bakker *et al*., 2016). One model, developed to assess the surface water-groundwater exchange flux at the contaminated site in Hagfors, utilized the lumped parameter recharge model LUMPREM (Doherty, 2021) for construction of input values with respect to the recharge package of MF6. Because the aquifer stresses studied in Alingsås were applied over timeframes too short for application with LUMPREM, recharge management was instead handled using FloPy. For the Hagfors model, history matching was conducted using PEST_HP (Doherty, 2020), and uncertainty analysis was performed using PESTPP-IES from the PEST++ suite (White, 2018; White *et al*., 2020). In the case of Alingsås, both history matching and uncertainty quantification were conducted using PESTPP-IES, managed through the Python library PyEMU (White *et al*., 2016). The forward models were initially

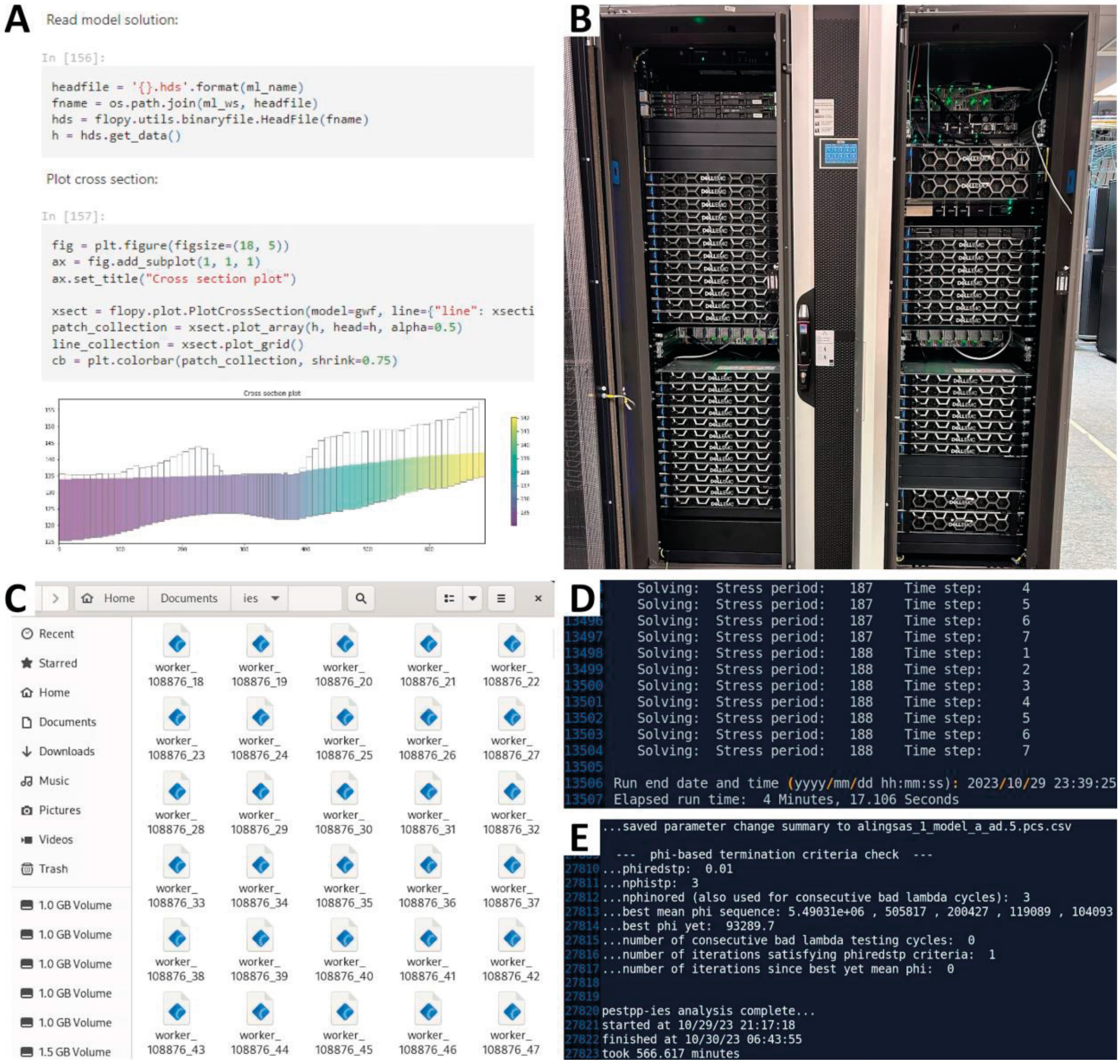

Figure 15. Details of the modelling workflow, showing A) model development and data analysis using Jupyter Notebook, B) a photograph showing a subset of the server racks hosting the LUNARC COSMOS (formerly LUNARC Aurora) HPC cluster (with permission from Anders Follin/LUNARC). C) depicts a screenshot from the login node showing multiple worker logs (one worker per CPU). D) shows records from a single worker log as it finishes one forward run, and E) shows records from the run manager upon completion after five iterations of history matching.

evaluated with a variety of parameter combinations to ensure reasonable numerical stability before commencing the more computationally expensive history-matching process. In the case of Alingsås, a prior Monte Carlo analysis using PESTPP-SWP (White *et al*., 2020) was undertaken, which helped to identify key areas for improvement and refine the model parameters for more accurate predictions. The spatial extent of the models' domains, as well as the mean of the prior parameter distributions, was determined based on existing information about the two sites. This information primarily came from well logs and slug test analyses and was supplemented by data from the hydraulic profiling tool, drill core logs, grain size analyses, older pumping tests, and 'best guesses' related to the geological setting.

The model run times varied from 4 to 8 minutes for the Hagfors model, and from 3 to 6 minutes for the Alingsås model. Because PEST calculates the Jacobian matrix in each iteration of history-matching by running the model as many times as there are adjustable parameters (PEST_HP) or model realizations (PESTPP-IES), this task is well-suited for parallelization. For this reason, LUNARC COSMOS, Lund University's high-performance computing (HPC; Fig. 15 B-C and Fig. 16) cluster, was leveraged to run the model in parallel, significantly facilitating the highly parameterized approach with 500 realizations in both models. Using the COSMOS HPC, up to five nodes equipped with 48 CPUs each were used, enabling up to 236 parallel model runs (four CPUs were dedicated to the run manager). PEST can be started in two modes: manager and worker mode. The run manager (Fig. 15 E) communicates with multiple workers via TCP/IP (one worker per CPU; see Fig. 15 C-D), providing instructions on which parameters (and observations, in the case of PESTPP-IES) to use in the forward run. The worker then returns the results of that specific forward run, enabling the manager to calculate the sensitivities for that element

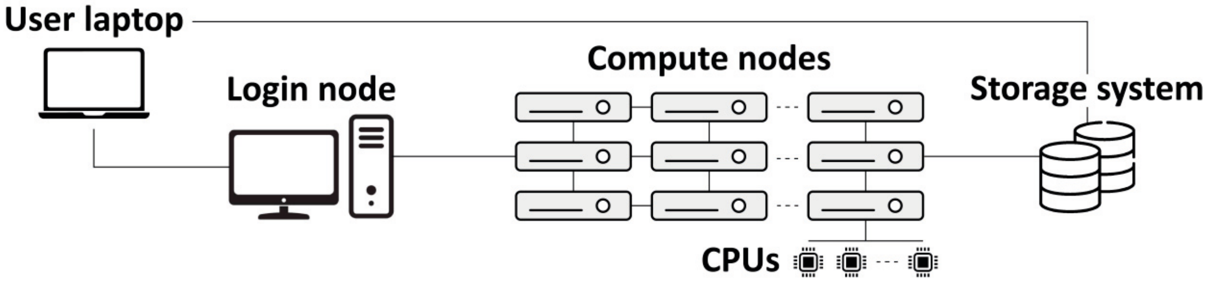

Figure 16. Workflow using the LUNARC COSMOS HPC cluster as approached in this thesis. The model design and architecture are constructed on a laptop using a platform-agnostic approach to ensure compatibility between Windows and Linux operating systems. The model is then packaged and compressed before being uploaded to the HPC cluster. Users manage the HPC system via a login node, from which they execute a batch program that transfers the model to the compute nodes. Each node processes the model in parallel, utilizing the number of CPUs assigned to each node. Upon completion, the results are uploaded to the HPC storage system, from which users can retrieve them.

in the Jacobian matrix. Once the Jacobian matrix has been filled, the iteration is complete. The run manager then begins to search the objective function surface to identify the steepest descent direction before commencing the next iteration. Upon completion, the results recorded by the run manager are transferred to the HPC storage system, from which they are retrieved for further analysis and postprocessing. This approach enables robust data assimilation while facilitating analytical work by distributing the computational load among multiple processors, leaving the workstation available for analytical tasks.

6 Results

This section summarizes the main findings of this doctoral thesis, based on the four papers that follow. The contributions of each author to these papers are detailed in Table 1. Additional results related to the findings in Paper II are presented in Section 6.2, expanding on the concepts discussed in this thesis.

6.1 Summary of papers

Paper I

Groundwater Modelling for Decision-Support in Practice: Insights from Sweden
Benavides Höglund, N., Sparrenbom, C., Barthel, R. & Haraldsson, E. (2024).
Accepted with minor revisions (June 2024).
Ambio. Under revision.

This paper examines the circumstances under which numerical groundwater models are used for decision-making support in the Swedish industry/Society. The motivation behind this investigation stems from a recent event where Sweden's largest cement producer was denied a permit renewal due to a 'bad model'. This denial could potentially result in the loss of over 200 000 jobs, significantly hamper national economic growth, and prompted the passing of a controversial amendment to the Environmental Code by the Swedish Parliament to circumvent the permit denial.

Our investigation is based on approximately one hundred reports that document the design and application of groundwater models in Sweden from 2010 to 2023. Our analysis reflects academic advances during this period and the current state of the art in the field. To complement this investigation and gain a broader understanding of practical applications within the industry, we have reviewed syllabi from water-related STEM courses in Swedish higher education. This review helps to assess the extent of groundwater modelling education and to establish a link between education and practice.

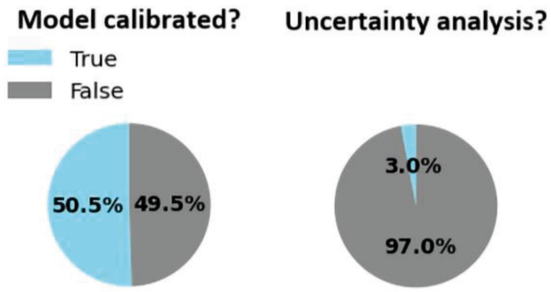

Figure 17. Approximately half of the models underwent some form of calibration, with the majority being manually calibrated through a 'trial-and-error' approach. Only a small minority of models, three percent, underwent uncertainty analysis, indicating that decisions based on most models were made without regard to the uncertainties accompanying the results. Modified from Paper I.

The results highlight a shortfall in uncertainty quantification relative to the objectives the models were designed to assess, significantly limiting the ability to provide decision-makers with clear metrics on model uncertainty (Fig. 17). In many cases, models calibrated against historical measurements suffered due to a small number of adjustable parameters and inflexible parameterization schemes. This likely hampered the calibration process, limiting the models' abilities to learn from data, which was often manifested in the form of poor fits with historical records of system state. These issues appear to reflect the insufficient inclusion of these concepts in groundwater education syllabi. Out of 83 courses where groundwater was a focus or the main subject, only two courses specifically focused on groundwater modelling, both emphasizing simulation with little or no inclusion of data assimilation or uncertainty analysis.

To address these issues, we presented suggestions for the industry, educational institutions, and decision-makers, which should be relevant not only in a Swedish context but also internationally. These suggestions include placing greater emphasis on groundwater modelling education, incorporating data assimilation and uncertainty quantification specifically in the syllabi to foster a holistic approach to decision-support modelling. Additionally, we suggested introducing numerical modelling early in projects, as it can help explore competing geological interpretations, thereby aiding in the formulation of data acquisition plans and potentially reducing project costs. Lastly, we promoted the implementation of flexible guideline recommendations for groundwater modelling. These recommendations should emphasize the integration of simulation, data assimilation, and uncertainty quantification, while also allowing for deviations when justified, thereby promoting robustness of model workflows while facilitating flexibility and the adaptation of new methods.

Paper II

A probabilistic assessment of surface water-groundwater exchange flux at a PCE contaminated site using groundwater modelling
Benavides Höglund, N., Sparrenbom, C. & Hugman, R. (2023).
Frontiers in Earth Science, 11.

This study examines the interaction between surface water and groundwater at the former Hagfors dry-cleaning facility. Remediation of this site has proven notoriously difficult, with numerous attempts over the years achieving only limited success. Because of this, the Swedish Geological Survey (SGU), the problem owner, decided to shift their focus to mitigating the discharge of contaminated groundwater into a nearby creek, which constitute the primary source of exposure in the area.

In this study, we constructed a model designed to quantify the surface water-groundwater exchange flux across the creek. The model was configured to simulate transient conditions under a four-year period (December 2015 to and including December 2019), using weekly time-steps. Recharge was simulated using LUMPREM (Doherty, 2021), which provided input for MF6. Surface water flow, including surface water-groundwater exchange flux was simulated and recorded using the Streamflow Routing (SFR) package of MF6. The model was calibrated using PEST_HP (Doherty, 2020), and predictive uncertainty was explored using PESTPP-IES. During history matching, a large number of observations (172 059) across a wide variety of observation types were assimilated. These included measurements of hydraulic head, stream stage, head-stage differences at locations using a dual-piezometer configuration, temporal-difference observations (synthetic datasets feature-engineered from the aforementioned measurements), temperature anomalies observed with fiber-optic distributed temperature sensing (FO-DTS) equipment, and expert knowledge. Assimilation of temperature anomalies and expert knowledge was configured using inequality-observations. Specifically, four areas where FO-DTS detected anomalously high temperatures, around 9°C compared to the ambient water temperature of approximately 4°C in December 2015, were identified as influx zones. Calibration targets were considered met when the simulation achieved any influx above zero in these areas. For expert knowledge, an inequality constraint ensured that calibration maintained continuous surface water flow from one SFR cell to its downstream neighbor throughout the model. This was necessary since initial calibration solutions suggested the creek could dry out under certain conditions, contradicting our knowledge of the site. The model workflow was designed to be reproducible, utilizing an online code repository which enabled interoperability across platforms and facilitated collaboration and transparency.

Predictive uncertainty was significantly reduced during history-matching. Because of this, our results allowed us to highlight specific locations where potentially contaminated groundwater is discharged into the creek. It also allowed us to provide an estimate of the rate of discharge, information valuable in the design of pump-and-treat systems for mitigating influx. These latter estimates differed significantly from previous estimates, which were based on steady-state model calibrated against approximately 30 measurements of hydraulic head using a trial-and-error approach, highlighting the value in assimilating time-series data across various types. Lastly, using surface water chemistry measurements, we estimated the yearly mass influx of dissolved PCE, which was found to be in broad agreement with previous estimates of the site.

Paper III

Multidisciplinary Characterization of Chlorinated Solvents Contamination and In-Situ Remediation with the Use of the Direct Current Resistivity and Time-Domain Induced Polarization Tomography
Nivorlis, A., Dahlin, T., Rossi, M., Höglund, N. & Sparrenbom, C. (2019).
Geosciences, 9.

This paper presents a multidisciplinary approach to characterizing the contaminated former laundry site in Alingsås, utilizing a combination of direct measurements and geophysical techniques. It focuses on the early results obtained from a novel method for monitoring the geophysical response to a pilot remediation campaign that was initiated in November 2017. During this campaign, two remediation fluids were injected at approximately thirty locations per fluid at the site: Provectus ERD-CH4™, containing a bacterial consortium and a carbon source, and CAT100™, containing zero-valent iron. The monitoring system used four layouts of permanently installed electrodes to enable time-lapse measurements of direct current resistivity and time-domain induced polarization (DCIP). The repeated measurements enabled the construction of DCIP tomographies in which the underground transport and possible biochemical changes of remediation fluids were observable. Additionally, two pairs of monitoring wells, equipped with cylindrical electrodes mounted on the outside, provided DCIP cross-hole tomographies. These tomographies revealed high-resistivity anomalies at locations where previous MIP measurements indicated the presence of DNAPL. Six lines of seismic refraction surveying was performed outside the facility to delineate the depth to the bedrock beneath the parking lot and support DCIP tomography interpretation.

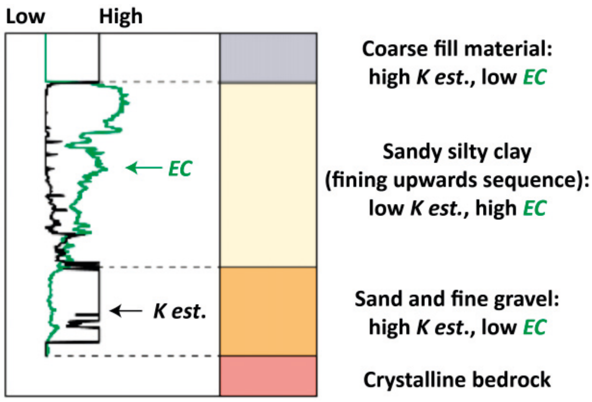

Figure 18. Interpretation of electrical conductivity response (*EC*; measured on the MIP) and estimated hydraulic conductivity (*K est.*; obtained from the HPT) in relation to the geology at the site, as described in various well log records. The fill material consists of coarse-grained, loosely packed particles indicated by low *EC* and high *K est.* The underlying unit, consisting of sandy silty clay, is characterized by high *EC* and low *K est.* As indicated by the decreasing *EC* towards the bottom, the clay content gradually decreases, why this unit is described as 'fining upwards'. An abrupt increase in *K est.* to values indicative of sand and fine gravel follow towards the bottom, where the probe hits impermeable crystalline bedrock. The truncated values in *K est*. provide the lower and upper bounds of the method presented by McCall & Christy (2010). Modified from Paper III (Nivorlis *et al.*, 2019).

Although the focus of this study is on geophysical method development, my contribution mainly involves the site description, geological interpretation, and figures related to them. Developing a comprehensive understanding of the site's geology was essential for providing a robust framework against which the geophysical data could be interpreted. The geological characterization primarily relied on historical well log records and an MIP/HPT campaign conducted earlier that year. Specifically, high-resolution vertical profiles of electrical conductivity and estimated hydraulic conductivity, measured with MIP and HPT respectively, provided detailed insights into the subsurface disposition. This information was correlated with lithological descriptions in the well log records, which served to categorize the subsurface into coherent lithological units (Fig. 18). Two cross-section profiles oriented perpendicular to the expected transport path of the plume, and one transect oriented along the expected direction of the plume were then created using this information. Results from the refraction seismic survey, historical well log records, and interpretations of MIP/HPT data served to inform the structural design of the model developed in Paper IV.

Paper IV

Assimilation and Worth of Injection Response Data for Enhanced Contaminated Site Characterization

Benavides Höglund, N., Sparrenbom, C. & Hugman, R. (2024).
Accepted with minor revisions (April 2024).
Hydrogeology Journal. Under revision.

Both site characterization and site remediation are costly endeavors and may require multiple campaigns if the underground is complex and/or the contaminant proves difficult to find and remove. This paper outlines a method for capturing and utilizing the hydrogeological response to a specific remediation technique, in-situ injection remediation, to characterize the subsurface and reduce parameter uncertainty.

Typically, hydrogeological parameters are estimated using mathematical models that evaluate the groundwater responses to various stresses. In-situ injection remediation is generally performed at many injection points across a site. Because the remediation fluids displace groundwater upon injection, this displacement and subsequent recovery can be regarded as a stressor. These events, therefore, present an opportunity to acquire spatially-distributed information on hydrogeological parameters that are valuable in the context of repeated remediation campaigns or in the formulation of a monitoring program. However, challenges regarding parameter estimation arise due to the high pressures involved during injection. Under these conditions, unconsolidated sediment may fracture, thereby temporarily or permanently increasing the bulk hydraulic conductivity to levels unrepresentative of in the undisturbed sediment. To explore different strategies in assimilating the response in hydraulic head observed during these events, we evaluated four structurally identical, but differently configured models. Two of the models utilized the Time-Varying Hydraulic Conductivity (TVK) and Time-Varying Storage (TVS) packages in MODFLOW 6 (MF6). These packages allowed for the adaptation of temporary parameter values, configured to act as multipliers on existing parameter values within a certain radius around each injection point. This setup allowed large deviations in parameter values that temporarily occur during hydraulic fracturing, as observed in the field when injectants surfaced through fractures around the injection points. The remaining two model configurations treated parameter values with respect to hydraulic conductivity and storage as temporally static fields, reflecting a more traditional setup. Two different configurations with respect to the weight of observations and their contribution to the objective function were also evaluated. One configuration treated both ambient observations and those recorded during injections as equally important; the other assigned greater importance to observations that deviated more from their mean observed value, implying that observations recorded during injections contributed more significantly to the objective function value.

Model performance was evaluated using two metrics: Parameter variance reduction (PVR) and prediction interval coverage probability (PICP). These metrics provided two valuable perspectives: PVR facilitated comparison between configurations in relation to apparent uncertainty reduction, and PICP enabled comparison of the models' abilities to replicate past system behavior. We found that PVR was highest in models configured to use neutral observation weights, but that PICP was highest in models that assigned greater importance to observations recorded during injections. Considering the higher accuracy in models that prioritized observations recorded during stress events, this suggests that PVR in neutral-weight models is likely inflated and therefore unreliable in terms of capturing nuances in injection data. The most accurate model configuration utilized time-varying parameters during injections in combination with a dynamic weighting strategy that prioritized observations from injection events.

A data worth analysis designed to compare the reduction in parameter uncertainty between ambient data and injection data was conducted on the best-performing model configuration. The analysis showed that injection data, collected over a few days, was both richer in information compared to the ambient data (collected over two months), as well as contained unique information pertaining to the injection area that was not present in the ambient data.

6.2 Findings outside publications: value of FO-DTS temperature anomalies

Assimilating temperature anomalies detected through FO-DTS during history-matching, as demonstrated in Paper II, represents a novel approach to reduce predictive uncertainty in models designed to quantify surface water-groundwater exchange fluxes. Quantifying this reduction in predictive uncertainty and analyzing how these temperature anomalies reduce uncertainties across space and time is a logical next step. By applying Equation 21 (through the Python library PyEMU) on the Hagfors model results obtained with PESTPP-IES, the worth of temperature anomaly observations can be quantified (Fig. 19, upper subplot). As shown, temperature anomalies may reduce uncertainties pertaining to surface water-groundwater exchange fluxes by up to 50 percent where observed. However, the value of these observations diminishes rapidly just a few meters downstream or upstream of these observed anomalies (the median uncertainty reduction is 0.7 percent).

The study period spanned from December 2015 up to and including December 2019, with the FO-DTS field campaign conducted in December 2015 (Sebök, 2016). This presents an opportunity to investigate how the value of these observations change over time, and whether they retain some of their value in the years that follow such a campaign (Fig. 19, lower subplot). As shown, even long after the temperature anomalies were observed, they continue to contribute significantly to reducing uncertainty at specific locations along the stream where detected. However, as the studied period progresses, this contribution become somewhat more erratic, coinciding with a relative reduction in predictive uncertainty and an increase in the relative importance of classical observations, such as hydraulic head.

7 Discussion and perspectives

The papers appended in this thesis are organized in a broad, holistic view of decision-support groundwater modelling, then move into specifics of how different types of data can be integrated to reduce predictive uncertainty. The first paper examines the practical applications of this modelling, focusing on the Swedish context but employing a wide lens by considering various sectors and linking with education through an analysis of groundwater-related course syllabi. The second paper presents a study that utilizes unconventional data to reduce uncertainties related to the surface water-groundwater exchange flux. My contribution to the third paper includes a geological site characterization using diverse, high-resolution datasets, which contributes to the structural design of the numerical models in the fourth paper. The latter paper evaluates different methods for reducing parameter uncertainties using injection-response

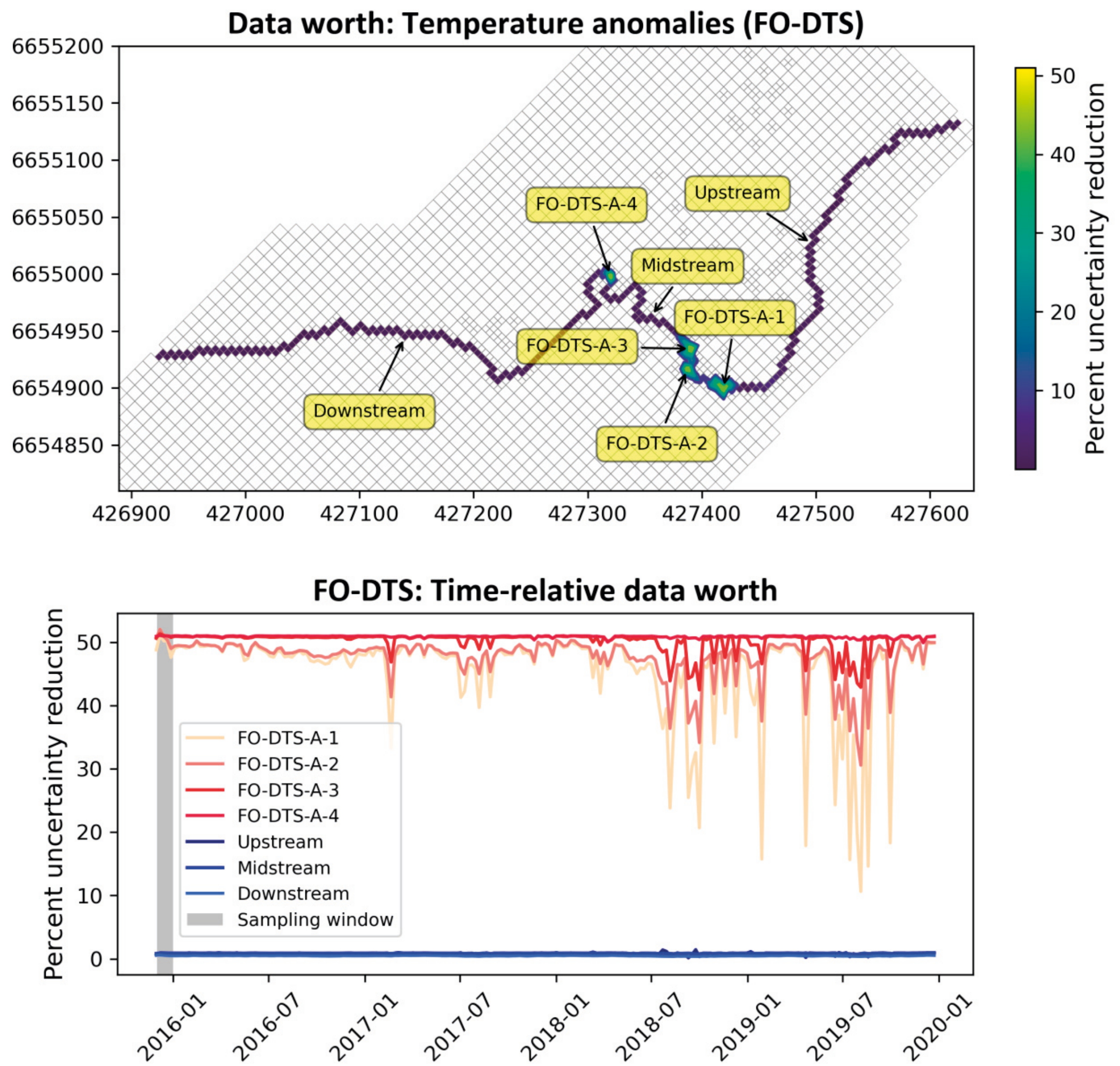

Figure 19. Worth of temperature anomalies in reducing uncertainty in surface water-groundwater exchange flux. The upper subplot displays the numerical model grid, with colored cells indicating the creek as defined by the SFR package in MF6. The map includes a marked 'Upstream' cell, positioned halfway between the first cell where inflow occurs and the cell where the initial temperature anomaly 'FO-DTS-A-1' is detected. Labels 'FO-DTS-A-2', 'FO-DTS-A-3', and 'FO-DTS-A-4' represent the remaining temperature anomalies, with labels 'Midstream' representing the position between 'FO-DTS-A-3', and 'FO-DTS-A-4', and 'Downstream' representing the position between 'FO-DTS-A-4' and the last cell where outflow occurs. The lower subplot highlights the worth of temperature anomalies during the time of detection ('Sampling window') as well as during subsequent time steps after removal of the FO-DTS equipment.

observations. The fourth paper, along with the results of an extended analysis of the site presented in the second paper, also expands upon the value of different types of data used in these types of studies. This section aims to complement the discussions in these papers by focusing on supporting information that was not primarily highlighted in these studies, and to integrate these insights at a higher level.

7.1 Challenges and opportunities facing applied decision-support groundwater modelling

A key discovery presented in Paper I is the significant discrepancy between important academic advances and the lack of integration of these concepts into education and practice. As exemplified by a recent and unusual case in the Land and Environmental Court of Appeals (LECA, 2021), insufficient modelling efforts can have detrimental effects on society, leading to environmental, financial and political repercussions. This unfortunate state is likely the result of a combination of multiple factors. However, to frame this discussion properly, a number of observations from Paper I are presented. First, it should be recognized that groundwater modelling is an established tool frequently applied to solve diverse groundwater-related issues within the industry. Indeed, many established consultancies were present in the dataset of model reports on which Paper I was based. Second, there exists, to some extent, a recognition among educational institutions of the importance of groundwater modelling. This is

Table 1. Contributions to the papers included in this thesis. Names in italic are not co-authors

	PAPER I	PAPER II	PAPER III	PAPER IV
Study design	**N. Benavides Höglund** C. Sparrenbom R. Barthel	**N. Benavides Höglund** C. Sparrenbom R. Hugman	A. Nivorlis T. Dahlin M. Rossi	**N. Benavides Höglund** C. Sparrenbom R. Hugman
Field work		**N. Benavides Höglund** *J. Jennerheim* *S. Åkesson*	A. Nivorlis M. Rossi	**N. Benavides Höglund** *J. Jennerheim* *J. Björn*
Data analysis and preprocessing	**N. Benavides Höglund** R. Barthel	**N. Benavides Höglund**	A. Nivorlis M. Rossi **N. Benavides Höglund**	**N. Benavides Höglund**
Modelling and postprocessing		**N. Benavides Höglund** R. Hugman		**N. Benavides Höglund**
Interpretation and discussion	**N. Benavides Höglund** C. Sparrenbom R. Barthel E. Haraldsson	**N. Benavides Höglund** C. Sparrenbom R. Hugman	A. Nivorlis T. Dahlin M. Rossi **N. Benavides Höglund** C. Sparrenbom	**N. Benavides Höglund** C. Sparrenbom R. Hugman
Figures, illustrations and tables	**N. Benavides Höglund**	**N. Benavides Höglund**	A. Nivorlis **N. Benavides Höglund**	**N. Benavides Höglund**
Writing: original draft	**N. Benavides Höglund** C.Sparrenbom	**N. Benavides Höglund**	A. Nivorlis T. Dahlin M. Rossi **N. Benavides Höglund** C. Sparrenbom	**N. Benavides Höglund**
Writing: review and editing	**N. Benavides Höglund** C. Sparrenbom R. Barthel E. Haraldsson	**N. Benavides Höglund** C. Sparrenbom R. Hugman	A. Nivorlis T. Dahlin M. Rossi **N. Benavides Höglund** C. Sparrenbom	**N. Benavides Höglund** C. Sparrenbom R. Hugman

demonstrated by the number of groundwater-related courses in which the syllabi mention groundwater modelling. It is also evident from the numerous master's theses on groundwater modelling written in collaboration with consultancies by students from science and engineering faculties at major Swedish universities. Thirdly, advances in decision-support modelling are often documented by people or teams that represent both researchers and industry professionals. Given these conditions, it is notable and concerning that important concepts such as data assimilation and uncertainty quantification have not been integrated into relevant courses or into an industry operating under the Environmental Code, which stipulates the use of the Best Available Technique (BAT).

Gaps between groundwater research, education, and industry have been identified by several authors before. For example, Sowby & Walski (2021) suggest that limited exposure to research among students and practitioners is a root cause for this issue, with a tendency to rely more on manuals, which condense some research into more digestible forms. Simmons *et al*. (2012) observe that some university curricula have not changed much in the last 40 years, even though the field of hydrogeology has evolved significantly during this time. They also note that the underutilization of unconventional data, such as environmental tracers, may unnecessarily limit model usability and reliability, arguing for a more widespread use of diverse information. Irvine (2018) emphasizes the importance of well-documented and accessible software tools in bridging research and practice, noting that licensing fees can be a significant barrier. Comments by these authors, and others, published in various groundwater-related editorials, indicate that this gap remains an issue today and is not unique to Sweden. The findings from our work on Paper I offer an opportunity to contribute to this discussion and provide further examples and insight to this topic. For example, due to the lack of established guidelines and only rudimentary recommendations from SGU, practitioners in Sweden are left without clear guidance or benchmarks for robust modelling practices. Under these conditions, both in Sweden and elsewhere, practitioners are likely to rely on 'what usually works' to ensure that their clients' environmental applications are approved. In the Swedish context, this is typically manifested by a single deterministic model utilizing a refined grid with numerous layers, bearing the visual appearance of a complex model, yet it often lacks effectiveness as a decision-support tool due to its inability to assimilate historical measurements and quantify model uncertainty. For example, calibration by trial-and-error, which still remain the dominant method for model calibration within the Swedish industry, can be described like traversing the surface of the objective function (see Fig. 9) without a map, only to stop when the time or budget runs out. Under the guidance of senior practitioners who adhere to the status quo, junior practitioners with little exposure to groundwater modelling literature are likely to follow the steps of their supervisors.

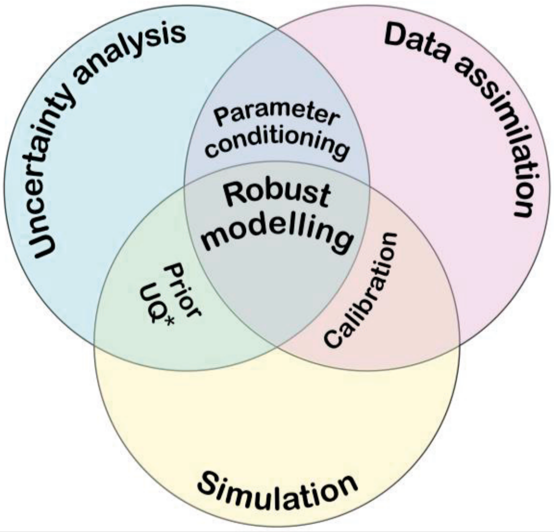

Figure 20. The three pillars of robust decision-support modelling, which include simulation, uncertainty analysis, and data assimilation, as illustrated in Paper I. Parameter conditioning is the process of conditioning parameter fields without requiring forward simulation of groundwater flow, for example, using multi-point statistics (MPS) or transition probability geostatistics (TPG). Prior uncertainty quantification (UQ*) serves to conduct Monte Carlo analysis without assimilating historical observations of system state, for example using PESTPP-SWP. In some cases, this approach may be sufficient. Prior UQ can also function as a diagnostic tool for models, providing practitioners with insights into potential model deficiencies.

Implementing guidelines for groundwater modelling is likely to enhance the quality and usefulness of models in the industry, though it also introduces some potential risks. For example, overly rigid guidelines could result in unnecessary work and increased costs, potentially leading to less frequent use of numerical models in favour of less effective tools. Additionally, these guidelines might foster a 'set it and forget it' mentality among the community and regulators, which could hinder the industry's adaptability to new advances and flexibility when needed. This is especially problematic in a fast-evolving field like numerical modelling, where new methods and best practices are frequently developed. For this reason, in Paper I, we propose implementing flexible guideline recommendations that may increase model quality and reliability while allowing for deviations when justified. In an attempt to condense the most important concepts in decision-support modelling, which are likely to remain relevant long into the future, a Venn diagram was created (Fig. 20) to illustrate these concepts and their interrelationships. Basing the guideline recommendations on these three concepts, rather than on one or multiple flow charts describing stepwise requirements, allows for greater flexibility among practitioners in tailoring the modelling to their specific cases. Reflecting principles of sound modelling, these concepts are central not only to process-based groundwater modelling but also to other forms of modelling, such as time-series forecasting. Of course, there may be benefits to standardizing certain approaches to modelling that relate to specific fields of application, as valuable insights can be gained from extensive experience in similar cases, such as those involving mining and tunnel construction. A reasonable approach to formulating guideline recommendations would be to establish a commission comprising representatives from industry, academia, and regulatory authorities. This commission could develop and oversee a 'living guideline document' that evolves and is maintained through a series of recurring workshops.

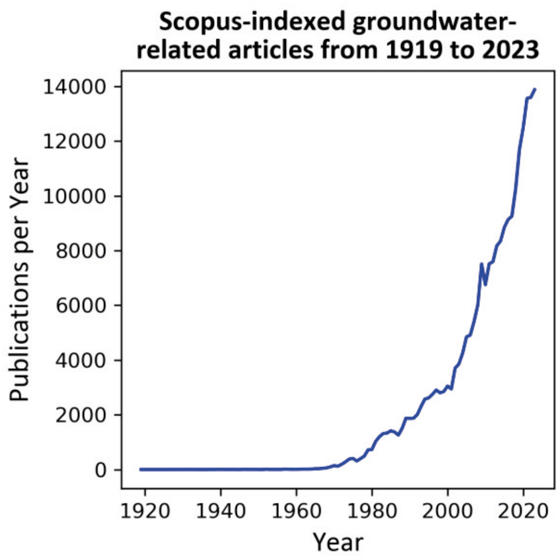

Figure 21. Scientific publications indexed annually in the Scopus Database (https://www.scopus.com, retrieved on 2024-06-04) that contain the word 'Groundwater' in their title, abstract, or keywords.

Of equal or greater importance to the implementation of guidelines is the integration of these concepts into groundwater education. Currently, groundwater-focused courses, to the extent that they cover groundwater modelling, tend to focus on simulation but overlook critical concepts like data assimilation and uncertainty quantification, which transform models into effective decision-support tools. Universities should provide a platform for current and future practitioners of groundwater modelling to learn from recent advancements in the field. Anecdotal observations from courses in related fields at the science and engineering faculties, where these concepts are integrated, can serve as a starting point for formulating such a course. Other suitable resources, based on well-documented open-source software, is discussed further in Paper I. As it stands today, students and practitioners have to reach out to courses offered abroad by foreign universities or private companies. Given the clear demand for competent groundwater modellers in the industry, the volume of groundwater modelling theses produced, and the current lack of essential concept integration in education, universities in Sweden and elsewhere, where these concepts are not integrated, should strive to enhance their education. According to Cherry (2023), groundwater education is our best means of combating the global water crisis, but it will require the recognition of leadership at universities to prioritize and invest in updated curricula and personnel. Groundwater models are our primary tools for assessing and quantifying groundwater related processes and issues, and a cost-effective suggestion for improving groundwater modelling education was presented in Paper I. Indeed, the timing for a renewed focus on these educational improvements is particularly suitable at this moment. As shown (Fig. 21), groundwater has gained significant focus among researchers over the past decades, reflecting an increased recognition of its importance in addressing water management challenges. Particularly in recent years, reports such as ‘Protecting Groundwater for Health’ (WHO, 2006), ‘Groundwater: Making the Invisible Visible’ (UNESCO, 2022), and ‘The Hidden Wealth of Nations: Groundwater in Times of Climate Change’ (The World Bank, 2023) confirms a widespread recognition among well-known NGOs of the importance of groundwater. Our environment and societies could greatly benefit if educational institutions were to align with this recognition and enhance their groundwater education.

7.2 Hydrogeological characterization using groundwater modelling and multiple lines of evidence

Characterizing the subsurface requires the collection and interpretation of data. Due to practical limitations and constrained budgets, we must prioritize the types of samples to collect, their quantity, and their locations. Once collected, interpretation may begin. This process typically involves the description and categorization of different lithological components based on various characteristics such as grain-size, mineralogy, texture and colour. Depending on sampling equipment and methodology, there may be information on properties invisible to the naked eye, such as electrical conductivity, permeability, or chemical composition. When comparing information from different sample locations, each property may be considered a single line of evidence among many that indicate the presence of a specific geological unit. The greater the alignment of evidence between two locations, the higher the confidence in interpreting lithological connectivity between these points. By connecting interpretations from multiple sample locations and multiple analyses and describing how they vary temporally and spatially, conceptual site models (CSM) in 2D and 3D can be developed. These models are important tools that facilitate discussions between stakeholders and enable communication between geoscientists, experts in other fields, and the public. They typically aim to capture the most prominent features of the subsurface but often generalize subjectively motivated ranges of natural variability into fixed categories. However, this generalization may downplay important nuances that play significant roles in hydrogeological contexts. Therefore, in terms of hydrogeological characterization, which takes into account the flow of groundwater through a site, CSMs are insufficient due to their static nature. This limitation is one of the many reasons why numerical models are commonly employed to simulate and quantify these dynamic processes.

As shown in the estimated K data recorded with the HPT probe (Fig. 18), used for the development of the CSM in Paper III, occasional spikes of higher hydraulic conductivity in the upper sandy silty clay were revealed. Although categorized as a single unit, these spikes indicate fractures (e.g. Fig. 13 D) within this lithological unit that, from a hydrogeological perspective, constitute preferential pathways for groundwater flow and solute transport. By contrast, the lower sedimentological unit, which contains sand and fine gravel, exhibits high values of estimated K with occasional ‘inverse spikes’, indicating interbeds of finer material. To describe the hydrogeological processes at this site, including any other site, the hydrogeologist is confronted with the subjective decision of determining which scales are important to represent and can be realistically captured by available data. In terms of groundwater numerical modelling, this consideration also includes factors of more practical nature such as numerical stability, model run time, and available disk space. In the case of the CSM developed in Paper III, the general characteristics of the sedimentological units, as shown in Figure 18, were observed in a majority of the sample locations. Given the small study area of the site in Alingsås, this is not surprising. However, depending on the sample location, these characteristics exhibited significant variability in terms of thickness, number of fractures, and presence of interlayering. For the purpose of supporting the geophysical interpretation of the DCIP tomographies presented in Paper III, the CSM which generalized these features into categories was sufficient. However, for Paper IV, which investigated the utilization and assimilation of injection-response data for hydrogeological characterization, representing the continuous variability of the underground was necessary. The decision on which scales to use in order to represent this variability, both spatial and temporally, was motivated by a number of factors. For example, the monitoring wells where transducers recorded pressure changes had filters spanning one or two meter intervals, varying by well.

Due to the length of these filters, they were likely to intersect one or several highly conductive fractures or less conductive fine-grained interbeds, depending on the depth at which the filters were positioned. This implies that even though the HPT data indicate the presence of highly variable hydrofacies at a fine scale, the calibration data recorded in the monitoring wells will reflect the bulk response over the entire filter length. Additionally, the temporal resolution of the recorded pressure data varied throughout the study period, necessitating a dynamic time-step configuration in the numerical models. This configuration was designed to capture detailed data during injections while ensuring sufficiently long intervals to record ambient dynamics in hydraulic head over approximately two months following the initiation of injection treatment. Under these settings, the design of the model grid, consisting of three layers, represented a subjective but necessary compromise. It considered the disposition of prominent sedimentological features, the positions and filter lengths of monitoring wells, the positions of injection points, the minimum bounding geometry of all pertinent site data, as well as model run time. In terms of hydrogeological characterization, the model assimilated field data through history-matching to provide estimates of hydrogeological properties, such as hydraulic conductivity and storativity, along with a range of uncertainty based on 500 model realizations. This number was chosen based on a compromise between available computational resources and model run time. These estimated properties are critical for any groundwater-related prediction aiming to explore the outcome of different management actions.

Similarly, the spatial and temporal discretization of the model used in Paper II was also motivated by a combination of factors relating to the required prediction, prevailing geology, data availability, and numerical efficiency. In the case of Hagfors, the prediction of management interest was the surface water-groundwater exchange flux. The most prominent geological feature was an elongated glaciofluvial deposit oriented NE-SW; the model grid was rotated to align with this orientation. Although occasional patches of tightly packed till are situated in topographic depressions at the bedrock interface, the creek flows through the glaciofluvial sediment, which is the dominant feature. Additionally, because the flux occurs surficially within the underground, the decision was made to represent the geology with a single layer. Because the characterization of the temporal dynamics of the surface water-groundwater exchange flux was a focus, the temporal discretization was set up to capture weekly time steps over a four-year period, spanning the bulk of available data. This characterization resulted in a detailed assessment of the flux, including related uncertainties based on 500 model realizations. Consequently, twelve segments with distinct flux behavior were identified, which decision-makers could use to prioritize targeted remediation treatments.

In the context of the title of this thesis, 'improved hydrogeological characterization using groundwater modelling and multiple lines of evidence', a discussion is warranted between the models presented in this thesis and current industry practices. The setups of both numerical models described above differ in a number of important ways from the average model designed for decision-support in the industry, as presented in Paper I. The most important distinction is the prediction-guided design, which aims to facilitate the assimilation of pertinent data to reduce predictive uncertainty. This approach aligns with decision-support modelling methods suggested in recent papers by numerous authors (e.g., Guthke, 2017; Ferré, 2017; White, 2017; Doherty & Moore, 2020). By contrast, the alternative approach emphasizes preserving as much structural detail from the CSM in the numerical model as possible, under the assumption that a model that more closely resembles reality holds greater predictive power than one that does not. Consequently, the 'industry approach' typically results in structurally complex models that may be troubled by long run times and numerical instability. If calibrated using a robust data-assimilation approach, these models require thousands of runs when history-matched over several iterations, which is time-consuming, making these considerations crucial. However, if calibrated by trial and error, as most 'industry models' are, run time and numerical instability present less of an issue, although this comes at the cost of a less reliable model. Another important distinction lies in how parameters are assigned to the model and the manner in which they are allowed to vary. As presented in Paper I, most 'industry models' utilize no more than 25 parameters, whereas the model in Paper II utilized more than 1700 parameters and the model in Paper IV, which relies solely on ensemble methods, utilized more than 200 000 parameters. This significant difference in parameter counts and types greatly distinguishes the two approaches in their ability to assimilate information from field data during calibration. Moreover, the types of calibration data used also differentiate these two approaches in that most 'industry models', to the extent that they undergo calibration, do so using only measurements of hydraulic head. By contrast, the models presented in this thesis utilize numerous types of data (multiple lines of evidence), as detailed in Table 2, which explains the different observation types used in the calibration of the Hagfors model. A final important distinction is the probabilistic approach adopted in the models presented in this thesis, as opposed to the deterministic approach typically employed by the industry. By accounting for competing interpretations (Fig. 22), parameter variability can be expressed in a way that reveals areas of high and low parameter uncertainty (refer to Paper IV for illustrations highlighting parameter uncertainty reduction). Consequently, by quantifying the outcome of a prediction using many equally probable model realizations (an ensemble), predictive uncertainty can be explored. Although there are ways to also explore

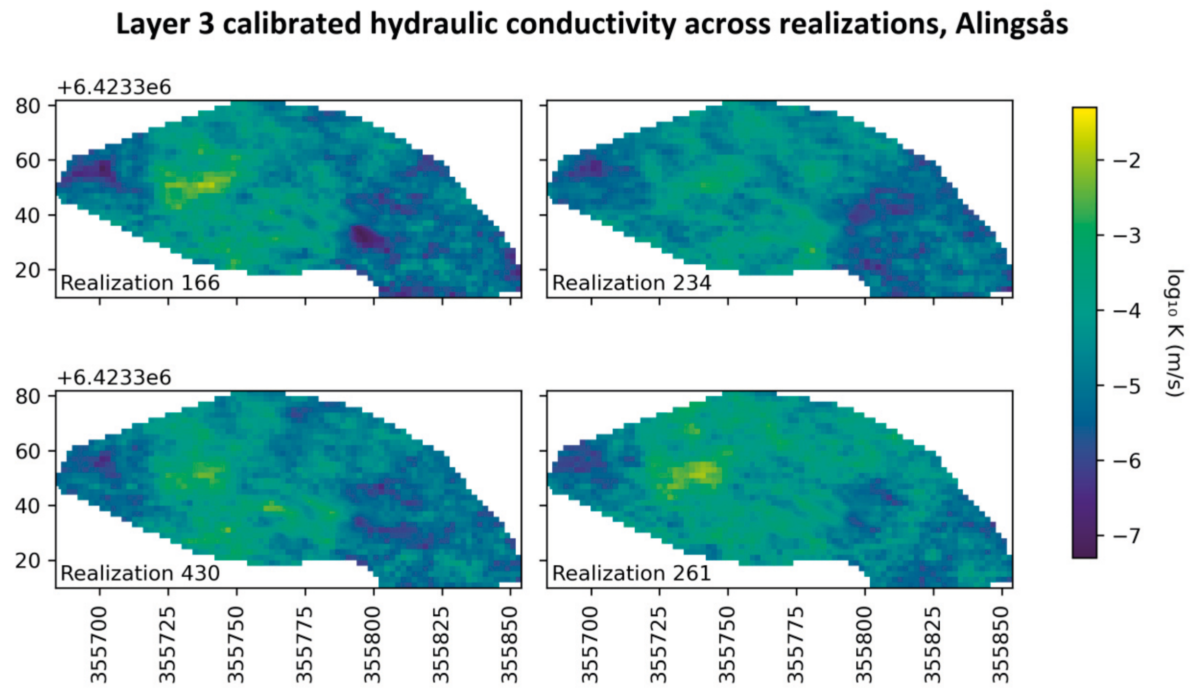

Figure 22. Competing interpretations of hydrogeological properties, as demonstrated through different model realizations. A total of 500 realizations were calibrated to fit the measured data within acceptable limits. Four of these are displayed here, each showing roughly similar characteristics but with individual distinctions.

predictive uncertainty using deterministic modelling, provided a Jacobian matrix is computed, the low number of parameters and the manual nature of trial-and-error calibration prevent this. This significantly limits the reliability of model results in 'industry models,' as the latter do not provide decision makers with an insight into the uncertainty of predictions. To maximize the insights gained from numerical models and to increase the likelihood that 'industry models' survive scrutiny from regulatory authorities, practitioners should update their modelling skillset based on recent advancements in this field. Some examples that can serve practitioners as a starting point were provided in Paper I.

7.3 Value of information

Continuing in the context of the title of this thesis, it is relevant to explore the value of the different lines of evidence used, with value defined as the extent to which specific observations, either individually or by type, contribute to reducing predictive uncertainty. Inherent in this statement is the insight that data worth is specific to the predictions the model is designed to make. This means that the same data is likely to be valued differently if the prediction is modified. As previously noted, most 'industry models', to the extent that they undergo calibration, rely solely on historical observations of hydraulic head. This reliance can likely be attributed to several factors. Firstly, groundwater observations are the most straightforward data to calibrate against in a groundwater model. Secondly, industry-standard GUI software is often designed with a bias toward this type of data, making it more challenging to incorporate other data types. Thirdly, practitioners may simply be unaware of the potential to calibrate models using other types of data. This subsection discusses the assimilation of various data types, as detailed in Papers II and IV, and how the industry could benefit from expanding its use of varied data sources.

The model developed in Paper II utilized eleven observation types (Table 2), of which five were synthetic datasets and two were configured as 'inequality observations' (calibration criteria are met above or below a set threshold). Classical observations include measurements of hydraulic head, stream stage, and stream flow rates. However, a novel type of observation, temperature anomalies, was also assimilated during history matching. These were set up as inequality observations at locations where warm water anomalies indicated an influx of relatively warmer groundwater. This means that the calibration criteria for these observations were met as long as an influx occurred at the time of detection, regardless of its size. As shown (Fig. 19), this information is highly valuable for reducing uncertainties related to surface water-groundwater exchange flux inside and near areas where such anomalies are observed, with the value persisting significantly into the future. It should be noted that this particular configuration, which uses inequality observations solely to identify an unspecified influx, represents a conservative application of the FO-DTS data. Several studies document the estimation of seepage rates directly from FO-DTS (e.g., Tristram *et al*. 2015; Le Lay *et al*. 2019). Using an approach that assimilates estimated seepage rates, including the forward propagation of any uncertainties in these estimates, would likely have increased the value of this data significantly compared

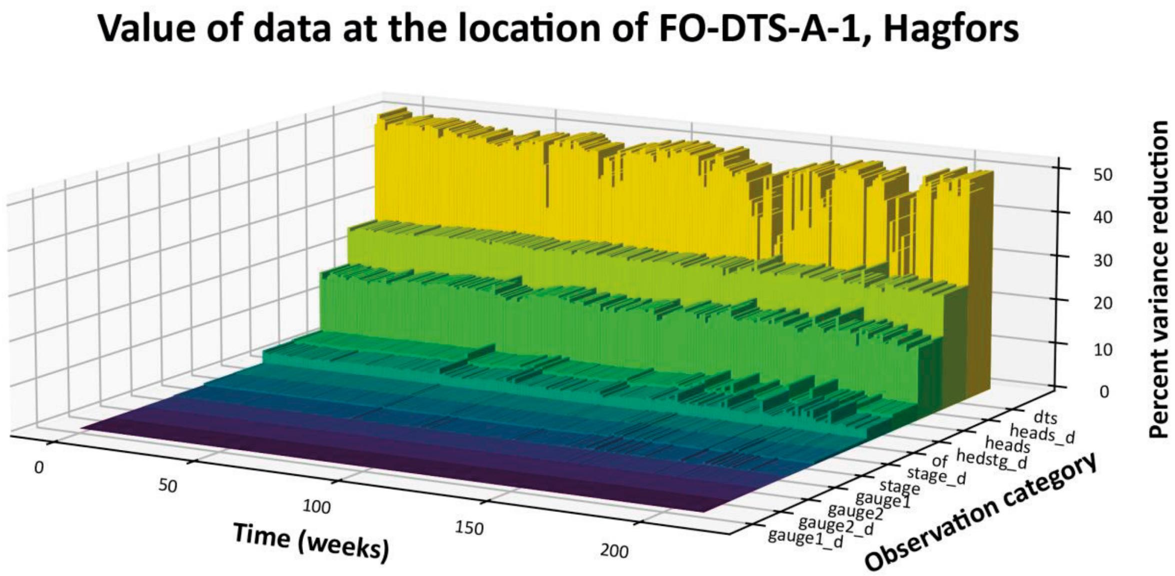

Figure 23. Data worth of different observation categories in terms of reducing predictive uncertainty at the location of FO-DTS-A-1 in creek Örbäcken, Hagfors. Refer to Figure 19 for details on the location. The categories and their contribution to the total percentage of observations are explained in Table 2. Each bar represents one timestep in the model, which pertains to one week. Week 1 corresponds to the first week of December 2015 and week 213 corresponds to the last week of December 2019.

to the setup described in Paper II, not only at the locations where these anomalies were observed but also along the entire FO-DTS coverage area. Extending the FO-DTS surveying campaign to capture temporal nuances over seasons would likely also enhance the value of this data, although the effectiveness of this method may be diminished as surface water and groundwater temperatures start to converge due to natural variations. Figures 23 and 24 illustrate the worth of all data assimilated during history-matching at two locations along the stream. At the location of an observed temperature anomaly (Fig. 23; see Fig. 19 for geographic details and Table 2 for an explanation of observation types), the value of the FO-DTS data approximately corresponds to the sum of all other observations combined. Upstream of this location (Fig 24), although the value of FO-DTS data is significantly lower, it still ranks among the most important observations. Notably, despite its relatively high value, the FO-DTS dataset constitutes a mere 0.02 percent of all observations assimilated in this model. The importance of synthetic datasets is also noteworthy. For example, the relative change in hydraulic heads over time (heads_d in Figures 23 and 24) contains more than twice the value of discrete measurements of hydraulic head in meters above mean sea level (heads) in terms of reducing uncertainty in surface water-groundwater exchange flux. This relationship is also observed with relative changes in stream stage (stage_d) compared to discrete measurements of stream stage (stage). The coupled surface water-groundwater transducer system (hedstg_d), which consists of five monitoring wells situated along the center of the creek at various locations, is also of relatively high importance. This system is equipped with one transducer inside the well to measure pressure changes in the groundwater and another transducer outside the well to measure pressure changes in the surface water. The dataset is derived from the difference between these pressure levels.

At the Alingsås site, the data worth analysis was designed to evaluate the same type of data, hydraulic head, although sampled under two vastly different settings. The study primarily focused on exploring different methods of assimilating injection-response data, which measures the response of hydraulic head to the injection of remediation fluids under high pressure. Here, the 'prediction' was more theoretical than practical, set to estimate key hydrogeological properties such as hydraulic conductivity, specific yield, and specific storage at the scale of the representative elementary volume (REV; see Fig. 4). Implicit in this approach is the assumption that these properties, and the uncertainties related to them, will have a significant impact on any prediction made by a groundwater model. The reader is referred to Paper IV for the results of this analysis, which compares the worth of hydraulic head measurements taken during the injection of remediation fluids and the subsequent hours of recovery with those taken under ambient conditions over approximately two months. Notably, this analysis highlights two important findings. Firstly, the injection-response data contains overall more detailed information on hydrogeological parameters compared to the ambient data. Given that this information includes data recorded during approximately sixty spatially distributed injection events, along with their subsequent recovery, this result is not surprising. Secondly, the injection-response data provides unique information specific to the areas where the injection treatment was performed, which is not available in the ambient data. Given that this area is likely of particular interest for any further treatment campaigns or future monitoring programs,

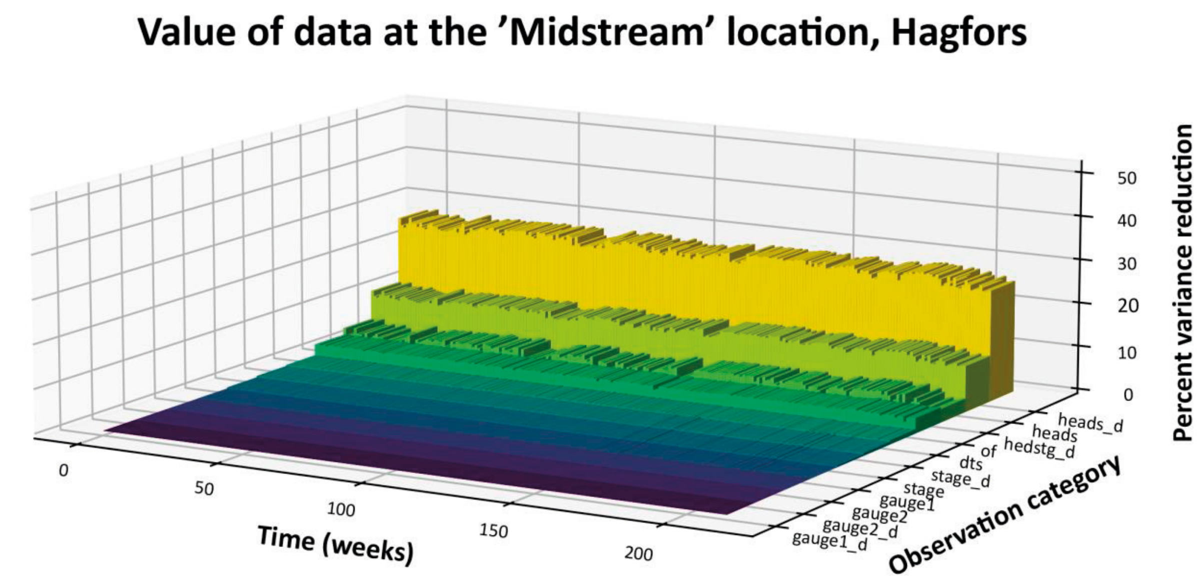

Figure 24. Data worth of different observation categories in terms of reducing predictive uncertainty at the 'Midstream' location, Hagfors. Refer to Figure 19 for details on the location. Note the rearranged order of observation categories compared to Figure 23, and that the worth of 'dts' is drastically lower compared to FO-DTS-A-1. Refer to Table 2 for an explanation of the categories. Week 1 corresponds to the first week of December 2015 and week 213 corresponds to the last week of December 2019.

the unique information contained in the injection-response data is especially valuable. Moreover, because this valuable information can be obtained without additional installations or special equipment, but simply by reprogramming the pressure transducers in existing monitoring wells to record at a higher frequency, it represents a cost-effective way to gather critical data. Based on our findings in Paper IV, we provided recommendations for sampling frequencies for this approach, suggesting at least one record per minute.

If the industry adopts more robust data assimilation strategies and complements groundwater numerical modelling with data worth analyses, it is likely to enhance practices, leading to improved modelling workflows and more effective data acquisition programs. Generally, consultancies possess a broad skill range and are proficient in collecting various types of data. However, insights from the combination of these sources of information may be diminished since they are not collectively integrated within a decision-support framework. Groundwater numerical models provide a framework where this information can be integrated through data assimilation to improve model reliability and reduce predictive uncertainty, as well as to inform what data will provide the most value. Schilling *et al*. (2019) provide a comprehensive overview on the use of unconventional observations in groundwater models, which could serve as a starting point for curious practitioners. However, more examples are needed in our field to serve as inspiration and to expand the body of knowledge regarding which types of data are worthwhile to collect under varying circumstances. Paper II and IV present insightful examples that likely challenge the prevailing line of thinking within the industry. These papers

Table 2. Explanation of the different observation categories and the percentage of total observations contributed by each group at the Hagfors site.

Observation category	Explanation	Percent of total observations
dts	FO-DTS temperature anomalies	0.02
heads_d	Hydraulic heads temporal difference (synthetic data)	14.6
heads	Hydraulic heads	14.72
hedstg_d	The difference between hydraulic head and stream stage measured at dual-piezometer monitoring stations (synthetic data)	3.79
of	Expert knowledge / outflow observations preventing simulated streamflow from drying out	51.77
stage_d	Stream stage temporal difference (synthetic data)	4.41
stage	Stream stage	4.42
gage1	Streamflow measured at the first gage	2.36
gage2	Streamflow measured at the second gage	0.78
gage2_d	Streamflow temporal difference (synthetic data)	0.78
gage1_d	Streamflow temporal difference (synthetic data)	2.36

demonstrate the relatively higher value of feature-engineered datasets (synthetic data) and temperature anomalies compared to conventional measurements of hydraulic head. Additionally, Paper IV illustrates how unique information can be obtained by tuning existing equipment to record the hydrogeological response during contaminated site injection treatments.

7.4 Future research

Although Paper I primarily focused on applied decision support modelling, it briefly explored groundwater-related syllabi and water operations cases at the Land and Environment Court of Appeals (LECA). In these cases, groundwater numerical models likely played a crucial role in the decision-making process. Specifically, seven cases were cited in which concerns about model uncertainties were raised. Decision-making within environmental courts would likely benefit from increased awareness of model capabilities, limitations and uncertainties (Rubin *et al*., 2018). Model predictions supplemented with assessments of uncertainty enable the quantification of risk, transforming it into a tangible factor around which risk-informed decisions can be made, rather than treating it as an abstract concept. To promote this increased awareness, establishing a baseline for how environmental courts currently handle model assessments would be beneficial. A systematic review of water operations cases within the Land and Environment Courts (LEC) could provide the necessary insights to form this baseline. To widen the scope and address groundwater-related uncertainty more comprehensively, it is suggested to include cases where either numerical or analytical models have been applied, as both types are relevant. However, accessing cases from the LECs, which are expected to contain a majority of the decided cases (with the LECA handling only appeals), is more challenging than searching the LECA database, which is publicly accessible online. The repositories of the five LECs can be searched only by their staff, and specific details such as case number or property number must be provided to facilitate these searches. With sufficient resources and potential collaboration with the LECs, this systematic review could likely be successfully accomplished.

Chlorinated solvents often present complex problems when spilled into the ground. Frequently, they are discovered decades after the spill occurred, and may be present in their original compound form, such as PCE or TCE, or as any of the metabolites. If the solvents are in the free phase, their transport may be density-driven along the slope of an impermeable surface or, if dissolved, in the direction of groundwater flow. Over time, the bulk mass may adsorb into the matrix of the soil and bedrock, making back-diffusion the primary method of transport. In the case of the Hagfors aquifer, once the discharge of contaminated groundwater into the creek has been mitigated, the problem owner's focus will shift to remediating the source zones. Drawing from the approach outlined by Pollicino *et al*. (2021), a groundwater model can be developed to estimate possible source zone locations and quantify their solute mass inflow rates through the assimilation of concentration data, which allows for the formulation of targeted remediation actions. Additionally, once ranges of these mass inflow rates have been quantified, an estimate of the total remaining mass can be back-calculated, facilitating the formulation of realistic remediation goals. Such a model assessment will benefit the remediation of the source zones at Hagfors, which have partly undergone transformation over the decades. It can be complemented with a data-worth analysis to reduce uncertainties regarding the source zone locations, thereby supporting effective remediation efforts.

Continuing the topic of groundwater modelling for forensic use at contaminated sites, results from the final fieldwork campaign at the Alingsås laundry in October 2020 challenged previous interpretations of the contaminant plume distribution. The prior extent of the plume, depicted in Paper III and in the technical reports cited therein, was primarily derived from the MIP campaign in 2017, which occurred before the remediation injection treatment. The plume is depicted as oriented NNW, following the slope of the crystalline bedrock situated below the unconsolidated sediment, and extending from the facility to beneath the parking lot. However, during the October 2020 fieldwork, the highest concentrations of PCE were detected outside this plume, approximately 50 meters west of it and in the general direction of groundwater flow, as indicated by the calibrated models in Paper IV. Because the MIP is expected to detect contaminants both dissolved in groundwater and adsorbed onto particles, the discovery of PCE rather than its metabolites this far from the source zone was puzzling, leading to the consideration of competing hypotheses. These include:

- A possible second source zone;
- Potential insufficiencies in the initial site characterization, predating our involvement at this site, which may have failed to accurately capture groundwater flow from the source;
- The likelihood that the injection of fluids during remediation could have mobilized the contaminant, pushing it away from the injection area to where it was found in October 2020.

A groundwater model could be developed using reverse particle tracking to assess the most likely hypothesis, following the approach of Hugman *et al*. (2023). This model could potentially identify additional areas at risk of contamination in this direction that may have been overlooked in previous site investigations, contributing to a more complete understanding of the situation at this site and enabling more successful remediation actions.

8 Conclusions

The scope of this thesis was twofold. Firstly, it aimed to investigate the practical application of groundwater modelling within the industry, establishing a link between industry and education, and analyzing this through the current state-of-the-art in the field. Secondly, the thesis explored methods to improve hydrogeological characterization through the use of groundwater modelling and multiple lines of evidence, with a focus on contaminated sites. Organized through three specific aims, this exploration included the collective assimilation of conventional data, unconventional data, and expert knowledge to reduce predictive uncertainty; the evaluation of different strategies for assimilating injection-response data during in-situ remediation treatments; and the quantification of the value of various types of data pertaining to their ability to reduce predictive uncertainty, including both conventional and unconventional data. The main conclusions of this thesis can be summarized as follows:

- Currently, applied groundwater modelling tends to emphasize simulation, overlooking essential concepts such as data assimilation and uncertainty quantification which bring worth to simulations in a decision-support context. Recognizing and incorporating these concepts into both industry practices and higher education is crucial for improvement in societal and environmental challenges.
- Groundwater models are applied to address a broad range of issues across various settings, including mining, tunnelling, water security, construction, and contaminated sites. However, the failure to properly assimilate relevant data or accurately represent critical processes may lead to criticism from regulatory authorities. These inadequacies may lead to environmental or financial damage, ultimately undermining the potential effectiveness of these models in decision-making processes.
- Implementation of flexible guideline recommendations for groundwater modelling that emphasize the integration of simulation, data assimilation, and uncertainty quantification can improve the reliability and applicability of models in decision-making processes. This approach ensures models are robust enough to withstand scrutiny and adaptable to new scientific advancements and varying project demands.
- The characterization of surface water-groundwater exchange flux along streams may be enhanced by applying groundwater numerical models to collectively assimilate various types of data containing information related to this process. Highlighted in a case study at a notoriously contaminated site in Sweden, this approach enabled the estimation of flux rates across the entire length of a stream and characterized their temporal variability over four years. Additionally, the analysis identified specific stream segments where potentially contaminated groundwater discharged, providing decision-makers with crucial information for targeted remediation efforts.
- Quantifying the value of different data types in terms of reducing predictive uncertainty is an important complement to regular model assessments. Specifically, in reducing uncertainties related to surface water-groundwater exchange flux, temperature anomalies indicating groundwater discharge are particularly valuable. These anomalies are estimated to be as valuable as all other observations combined where identified. Additionally, datasets featuring relative changes, for example in hydraulic head or stream stage, appear more valuable than those providing discrete measurements in meters above sea level, underscoring the importance of feature engineering.
- Capturing the hydrogeological response to the injection of remediation fluids underground presents a promising method for obtaining data rich in information on hydrogeological parameters. However, to mitigate the risk of introducing parameter bias due to the high pressures involved, which may fracture the subsurface, careful consideration must be given to how the injection-response data are assimilated. For example, using time-varying parameters within a radius around each injection point can help address this issue.
- A data worth analysis shows that the injection-response data contains more information on hydrogeological parameters compared to the information from two months of ambient groundwater measurements. Additionally, the injection-response data provides a higher level of detail regarding these parameters in the area where injections were performed, information which is absent in the ambient data alone. Because capturing this data only requires reprogramming pressure transducers to record the high-frequency response during injections, this approach provides a cost-effective way to gather critical information.

Popular summary

Contaminated sites present a global issue that manifests at the local scale. In Sweden alone, more than 80 000 contaminated sites have been identified. These sites pose a risk to human health, the environment, and essential resources like freshwater.

Groundwater is our largest liquid freshwater resource. It forms as rain and melting snow seeps into the ground, saturating the space between grains and cracks in the underground, a process known as groundwater recharge. Although it remains largely invisible in our everyday lives, we depend on it for our development and well-being. Approximately half of the world's population relies on groundwater for drinking water, hygiene, and cooking. It is also extensively used in irrigation, sustaining food production on a global scale. Additionally, groundwater supports terrestrial ecosystems and provides the base flow necessary to sustain aquatic life in many rivers and streams. With increasing pressure on our limited surface waters, groundwater will become even more crucial for supporting future sustainable development.

Just like the wind, groundwater moves from areas of high pressure to areas of low pressure. However, instead of flowing through the atmosphere, groundwater flows through the cracks and pore spaces within rocks and sediment beneath our feet. Understanding the rate of groundwater recharge, as well as the direction and velocity of its flow, is important in many different environmental and engineering applications. For example, this information helps determine sustainable extraction rates, delineate source water protection areas, manage dewatering in mining areas and tunnels, and address contaminated site cleanup.

The geoscientist's approach to interpreting and enhancing our understanding of the subsurface, including how groundwater flows through it, is by constructing models. A model can be a sketch on a piece of paper, a miniature physical model, a 3D rendering on a computer, an analytical model solvable by pen and paper, or a numerical model capable of simulating and quantifying natural processes. The latter category is extensively used in both industry and academia worldwide to quantify and predict the outcomes of various scenarios. This is also the category of models that this thesis focuses on.

When interpreting the disposition of the underground, we always operate under an information deficit. In general, our primary means of directly observing the composition and structure of the underground involves extracting cores and examining outcrops. Other techniques, such as geophysical methods, allow us to indirectly infer the properties of the underground without directly sampling them, similar to how a doctor examines a patient using X-rays. However, even with the most generous of budgets, the volume of the underground that remains unsampled far outweighs the sampled volume. Because of this, we must allow for competing interpretations as we describe the underground and processes therein, such as groundwater flow. Adopting a modelling approach that explores multiple competing interpretations, is therefore essential, as opposed to a traditional approach that only focuses on a single interpretation.

Although all models are uncertain, we can often reduce a meaningful amount of uncertainty by calibrating our models so that their simulated values match historical measurements from the field. If we approach this process carefully, the model can express important properties of the underground and pinpoint where this information is more certain or less certain. This is useful because it allows us to focus on areas that need further investigation or improvement. Sometimes, by calibrating our models using multiple types of data (multiple lines of evidence), we can reduce model uncertainty by a substantial amount.

This thesis is composed of four research papers. The first paper explores applied groundwater modelling for decision support in Sweden, examining reports that document the use of these models from 2010 to 2023. Additionally, to establish a link between practical applications and education, we investigate the extent to which groundwater modelling is incorporated into the curricula of Swedish higher education institutions. The results show that groundwater modelling is a low priority among groundwater-related courses and that important advances in the field have not been incorporated into these courses. Consequently, the industry tends to utilize ineffective techniques, often with little or no consideration for model uncertainty and competing interpretations. To improve the current situation, we offer distinct recommendations aimed at the industry, educational institutions and decision-makers. These recommendations include the incorporation of new and effective model workflows in both education and practice, as well as the formulation and implementation of official guideline recommendations grounded in robust methods.

The second paper addresses a contaminated site in Hagfors, Sweden, where approximately 120 kg of perchloroethylene, a substance highly suspected of being carcinogenic, leaks into a creek from contaminated groundwater each year. The creek flows through a sparsely populated area before entering a lake downstream. Reducing, or preferably stopping, the leakage of contaminated groundwater into the creek is a priority at this site. However, achieving this requires an understanding of the locations and rates at which the leakage occurs. We constructed a model designed to quantify the exchange of water between surface water flowing in the creek and the underlying contaminated groundwater. The model was calibrated using various types of data, including surface water measurements and groundwater measurements.

Additionally, a novel type of data, warm-water anomalies, was used to identify leaks of relatively warmer groundwater (approximately 9°C) compared to the colder surface water (approximately 4°C) in December 2015, detected using fiber optics. The calibrated model pinpointed specific locations where potentially contaminated groundwater leaked into the creek from below. By analyzing model uncertainty, we calculated a range of likely leakage rates, providing decision makers with insights into the volumes of potentially contaminated water that may need treatment, allowing for appropriate scaling of remediation efforts.

The third paper presents a new method for near real-time monitoring of cleanup efforts at contaminated sites. The method was tested at a site contaminated with perchloroethylene located in Alingsås, Sweden. This geophysical approach involves inducing an electrical current through the ground using electrodes and measuring its electrical resistivity. The variations in resistivity of the materials beneath the ground surface can be used to create cross-sectional tomographies of the subsurface. The monitoring system was installed prior to a cleanup campaign which utilized injections of fluids designed to stimulate breakdown of the contaminant. Through repeated measurements following this campaign, movement of the fluids through the subsurface was observable, thereby providing insights into the efficiency of the cleanup. As a co-author of this paper, my contribution focused on the geological interpretation of the site. When performing geophysical measurements like those described above, it is crucial to understand the geology through direct observations, such as information from boreholes, to establish a relationship between the geophysical response and the observed geology. To aid this process, I used historical records of direct measurements to construct 2D conceptual models of the geology, which facilitated the geophysical interpretation.

The fourth paper revisits the site in Alingsås, now focusing on the properties of the underground that control groundwater flow. The effectiveness of a groundwater model relies on how well it can accurately represent the physical properties at the scale needed for making predictions. Traditionally, determining properties like sediment permeability requires direct action, such as pumping and then measuring the recovery of groundwater after the pumping stops. These investigations are often costly and time-consuming. However, the fluids injected to clean up a site can also displace the groundwater, and this displacement and recovery can be used to estimate these properties. By leveraging these existing events, we can gather valuable information without additional expensive and time-consuming fieldwork. To explore the best way to extract this information, we designed four models, each configured differently in how they handled high pressures from injections and which measurements to prioritize during calibration. We found that the model which focused on observations recorded during high-pressure events and adjusted for the extreme pressures around each injection point provided the most reliable results.

In addition to the findings presented in the second and fourth papers, I analyzed the value of the data used for calibrating the models. By evaluating the 'data worth' based on how much each type of data reduces model uncertainty, we can compare different data types. This information is valuable for planning new data acquisition campaigns and facilitating cost-effective fieldwork.

In conclusion, the findings of this thesis highlight important challenges and provide suggestions for their improvement with regards to increasing the quality of decision support modelling both in education and industry. Furthermore, it explores creative ways to extract the most from data to enhance hydrogeological understanding, with a focus on contaminated sites. These methods have the potential to increase the effectiveness of site cleanup programs and reduce costs.

Populärvetenskaplig sammanfattning

Förorenade områden är ett globalt problem. Bara i Sverige har över 80 000 potentiellt förorenade områden identifierats. Dessa föroreningar kan spridas genom marken till grundvattnet och utgör därför en risk för hälsa och miljön.

Grundvatten utgör med god marginal jordens största tillgängliga färskvattenresurs. Även om grundvattnet är osynligt i vår vardag, är vi beroende av det för flera livsnödvändiga samhällsfunktioner, både för konsumtion och för samhällelig och ekonomisk utveckling. Globalt är ungefär hälften av världens befolkning beroende av grundvatten för dricksvattenförsörjning, samt för matlagning och hygien. Även i Sverige är ungefär hälften av alla hushåll beroende av grundvatten för sina dagliga vattenbehov. Grundvattnet har också en omfattande betydelse för den globala livsmedelsproduktionen, inte minst som en källa till bevattning. Utöver dessa direkta och indirekta kopplingar till människor och samhälle, utgör grundvatten en viktig del av vattenbalansen. Det bidrar till exempel till tillrinningen till våra vattendrag, vilket motverkar torrläggning även under längre torrperioder.

Grundvatten bildas när regn och smältvatten infiltrerar ner genom marken och mättar de porutrymmen som finns mellan mineralkorn och i sprickor i sediment och berg. Grundvattnet rör sig, precis som vinden, från områden med högt tryck till områden med lågt tryck. Men till skillnad från vinden, som förflyttar sig snabbt genom atmosfären, flyter grundvatten genom sprickor och porutrymmen i berg och sediment under marken. Denna process är mycket långsam och kan variera från veckor upp till tusentals år eller längre. Att utveckla en förståelse för grundvattenbildningens omfattning, såväl som för grundvattnets flödesriktning och flödeshastighet, är avgörande för att kunna lösa många miljötekniska problem. Exempel där sådan kunskap är avgörande inkluderar säkerställande av hållbar dricksvattenförsörjning, utformning av vattenskyddsområden, planering och bortledning av vatten vid gruvverksamhet eller tunnelbyggen, samt planering och genomförande av sanering av förorenad mark.

Som geovetare utvecklar vi ofta modeller för att tolka och förbättra vår förståelse av geologin och grundvattnets rörelser genom marken. En modell kan till exempel vara en skiss på en papperslapp, en fysisk modell i miniatyr, en konceptuell modell framarbetad i ett datorprogram, en analytisk modell som kan lösas med papper och penna eller en numerisk modell som kan simulera och beräkna olika naturliga processer. Den sistnämnda kategorin används ofta inom både branschen och forskning världen över för att beräkna utfallet av olika scenarier. Det är också den kategori av modeller som denna avhandling bygger på.

När vi arbetar med geologisk tolkning råder det alltid brist på information. Våra främsta metoder för att undersöka geologins sammansättning och struktur är att studera och provta borrkärnor eller blottlagda ytor, till exempel i stenbrott, vägskärningar eller naturligt förekommande erosionsytor. Men även med de mest tilltagna budgetar kommer vi bara kunna undersöka en bråkdel av den totala volym under marken som utgör vårt undersökningsområde. Vi behöver därför ta hänsyn till alternativa tolkningar när vi beskriver geologin och de processer som påverkas av dess utformning, till exempel grundvattnets flöde. För att ge plats åt alternativa tolkningar när vi utvecklar våra modeller, behöver vi använda metoder som bygger på sannolikhet, snarare än bestämdhet. Genom att kalibrera ett större antal *sannolika* modeller, snarare än en enskild modell, kan vi både sänka osäkerheten i våra beräkningar, men också få en uppfattning om hur mycket osäkerheten varierar på olika platser och under olika förutsättningar. Denna kunskap bidrar till att vi kan utforma mer effektiva och mindre kostsamma undersökningar av de förorenade områden som kräver sanering. Genom att använda modeller som ett verktyg för att sammanställa information från många olika typer av undersökningar ('multiple lines of evidence') kan vi förbättra vår förståelse av marken och grundvattnets rörelser avsevärt.

Denna doktorsavhandling består av fyra artiklar. I den första artikeln undersöker vi hur branschen använder grundvattenmodellering som ett verktyg för beslutsstöd i Sverige, genom att granska över hundra rapporter som dokumenterar användningen av modeller på olika platser från 2010 till 2023. För att utveckla vår analys undersökte vi även i vilken utsträckning grundvattenmodellering ingår i svenska lärosätens kursplaner. Resultaten visar att grundvattenmodellering är lågt prioriterat i de kurser som omfattar grundvatten i Sverige och att viktiga metoder inte ingår i de kurser som erbjuds. I och med detta tenderar branschen att använda ineffektiva arbetsmetoder, ofta utan att ta hänsyn till osäkerheter och alternativa tolkningar av grundvattnets rörelse. För att främja användandet av grundvattenmodeller och bidra till en förbättrad förståelse och nyttjande av data utformar vi ett antal rekommendationer som riktar sig till branschen, lärosäten och beslutsfattare. Vi rekommenderar att både branschen och universiteten som utbildar inom grundvatten anammar nya arbetsmetoder som tar bättre hänsyn till de osäkerheter som förknippas med modellering, eftersom detta främjar en öppnare, ärligare och mer informerad diskussion mellan beslutsfattare. Dessutom föreslår vi att riktlinjer för grundvattenmodellering som baseras på dessa metoder införs för att förbättra kvaliteten och tillförlitligheten i de beräkningar som påverkar beslut om grundvattnet.

Den andra artikeln avhandlar ett förorenat område i Hagfors. Här läcker cirka 120 kg perkloretylen, ett misstänkt cancerframkallande ämne som används inom kemtvättsverksamheter, in i en bäck från det förorenade grundvattnet varje år. Bäcken rinner genom ett glesbefolkat område innan den mynnar ut i sjön Värmullen nedströms. Efter att ha stött på stora svårigheter med att sanera föroreningskällan har SGU tillfälligt valt att prioritera att minska inläckaget av förorenat grundvatten till bäcken. För att uppnå detta mål behöver en förståelse för utbytet mellan ytvattnet och grundvattnet etableras. Vi utvecklade därför en modell för att i både tid och rum simulera och beräkna vattenutbytet mellan ytvattnet i bäcken och det förorenade grundvattnet. Modellen kalibrerades med hjälp av olika datatyper, inklusive ytvattenmätningar och grundvattenmätningar. Därutöver användes mätningar av temperaturskillnader i bäcken för att identifiera inläckageområden med relativt varmare grundvatten (cirka 9°C) jämfört med det kallare ytvattnet (cirka 4°C), vilket mättes med en fiberoptisk kabel i december 2015. De kalibrerade modellerna identifierade flera platser längs med bäcken där potentiellt förorenat grundvatten läckte in, och genom att använda många alternativa tolkningar av markens egenskaper, beräknade vi intervall för sannolika inläckageflöden. Dessa beräkningar hjälper beslutsfattare förstå vilka volymer av potentiellt förorenat vatten som kan behöva behandlas, vilket främjar planering och implementering av riktade saneringsåtgärder.

I den tredje artikeln presenteras en metod för att övervaka förloppet av pågående saneringsåtgärder genom att använda geofysiska undersökningsmetoder. Metoden utvärderades vid Västra Götalandsregionens tvätterianläggning i Alingsås, som någon gång innan millennieskiftet förorenats med perkloretylen. Metoden innebär att elektricitet leds genom marken med hjälp av elektroder för att på så vis mäta markens ledningsförmåga. Hur väl ström kan ledas genom undermarken beror bland annat på vilka slags jordarter och sediment som finns där, samt vid vilket djup grundvattenytan befinner sig på. Metoden kan, likt en röntgenplåt, ge en avbild av hur undermarken ser ut. Övervakningssystemet installerades strax innan saneringsåtgärder påbörjades under hösten 2017, då saneringsvätskor injekterades för att stimulera nedbrytning av föroreningarna. Genom att utföra upprepade mätningar kunde flödet och transporten av vätskorna genom marken observeras, vilket ökade förståelsen för hur väl saneringsvätskorna nådde ut i de förorenade massorna. Som medförfattare till denna artikel fokuserade jag på den geologiska tolkningen av området. För att dra största möjliga nytta av geofysiska undersökningar, är det viktigt att komplettera den geofysiska informationen med direkta observationer av geologin, såsom information från borrhål. Detta är nödvändigt för att fastställa ett samband mellan geofysiska data och den observerade geologin. Jag sammanställde därför information från borrhålsbeskrivningar från samtliga undersökningar gjorda på platsen de senaste tjugo åren, vilket underlättade det geofysiska tolkningsarbetet.

Den fjärde artikeln avhandlar också det förorenade området i Alingsås, men med fokus på de egenskaper i marken som styr grundvattnets flöde. En grundvattenmodells förmåga att göra användbara prognoser beror på hur väl modellen kan representera undermarkens egenskaper. För att beräkna dessa krävs vanligtvis att man påverkar grundvattnet, till exempel genom att pumpa, och mäta grundvattenytans avsänkning. Hur och var avsänkningen sker beror på markens egenskaper, varför dessa egenskaper kan härledas genom påverkan på grundvattnet. Sådana undersökningar är dock ofta både kostsamma och tidskrävande. Men eftersom saneringsvätskor, när de injekteras i marken, också tränger undan grundvattnet, kan man passa på att mäta hur grundvattenytan påverkas samtidigt som vätskorna injekteras. På så vis kan man utnyttja en redan pågående åtgärd för att utvinna värdefull information om undermarkens egenskaper som annars skulle kräva ytterligare kostsamma och tidskrävande insatser. För att undersöka hur denna information kan utvinnas på bästa sätt utvecklade vi fyra grundvattenmodeller med olika konfiguration. Undersökningen visade att den modell som lade extra vikt vid de mätningar som noterats under själva injekteringstillfällena, samtidigt som den kompenserade för de höga tryck med vilken saneringsvätskorna injekterades, var mest tillförlitlig.

Utöver de resultat som presenteras i den andra och fjärde artikeln har jag även utfört datavärdesanalyser för att undersöka vilken slags information som är viktigast att inhämta för att besvara olika grundvattenrelaterade frågeställningar. Informationsvärdet för olika datatyper har bedömts genom att undersöka hur mycket varje enskild datatyp bidrar till att sänka osäkerheten i de modellberäkningar som gjorts. Till skillnad från branschen, som oftast bara kalibrerar modeller med grundvattennivåer, visade analysen att det också är mycket viktigt att använda andra typer av data, såsom ytvattenflöden, ytvattennivåer, temperaturskillnader, samt 'mjuka data' så som expertkunskap.

Sammanfattningsvis lyfter denna avhandling fram flera viktiga utmaningar inom fältet. För att möta dessa utmaningar presenteras förslag på hur vi kan höja kvaliteten på de beslutsstödsmodeller som branschen utvecklar, genom att redan under utbildningen introducera viktiga koncept som idag saknas. Därutöver presenteras ett par kreativa metoder för att utvinna så mycket information som möjligt från olika typer av data för att förbättra geologiska grundvattenmodeller, med fokus på förorenade områden. Dessa metoder bidrar till mer riktade saneringsåtgärder och effektivare övervakningsprogram, och har därigenom potential att både öka effektiviteten och minska kostnaderna förknippade med efterbehandling av förorenad mark.

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