Probabilistic Contaminant Source Assessment

A GMDSI worked example report

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Groundwater Modelling Decision Support Initiative

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PREFACE

The Groundwater Modelling Decision Support Initiative (GMDSI) is an industry-funded and industry-aligned project focused on improving the role that groundwater modelling plays in supporting environmental management and decision-making. Over the life of the project, it will document a number of examples of decision-support groundwater modelling. These documented worked examples will attempt to demonstrate that by following the scientific method, and by employing modern, computer-based approaches to data assimilation, the uncertainties associated with groundwater model predictions can be both quantified and reduced. With realistic confidence intervals associated with predictions of management interest, the risks associated with different courses of management action can be properly assessed before critical decisions are made.

GMDSI worked example reports, one of which you are now reading, are deliberately different from other modelling reports. They do not describe all of the nuances of a particular study site. They do not provide every construction and deployment detail of a particular model. In fact, they are not written for modelling specialists at all. Instead, a GMDSI worked example report is written with a broader audience in mind. Its intention is to convey concepts, rather than to record details of model construction. In doing so, it attempts to raise its readers' awareness of modelling and data-assimilation possibilities that may prove useful in their own groundwater management contexts.

The decision-support challenges that are addressed by various GMDSI worked examples include the following:

- assessing the reliability of a public water supply;
- protection of a groundwater resource from contamination;
- estimation of mine dewatering requirements;
- assessing the environmental impacts of mining; and
- management of an aquifer threatened by salt water intrusion.

In all cases the approach is the same. Management-salient model predictions are identified. Ways in which model-based data assimilation can be employed to quantify and reduce the uncertainties associated with these predictions are reported. Model design choices are explained in a way that modellers and non-modellers can understand.

The authors of GMDSI worked example reports make no claim that the modelling work which they document cannot be improved. As all modellers know, time and resources available for modelling are always limited. The quality of data on which a model relies is always suspect. Modelling choices are always subjective, and are often made differently with the benefit of hindsight.

What we do claim, however, is that the modelling work which we report has attempted to implement the scientific method to address challenges that are typical of those encountered on a day-to-day basis in groundwater management worldwide.

As stated above, a worked example report purposefully omits many implementation details of the modelling and data assimilation processes that it describes. Its purpose is to demonstrate what can be done, rather than to explain how it is done. Those who are interested in technical details are referred to GMDSI modelling tutorials. A suite of these tutorials has been developed specifically to assist modellers in implementing workflows such as those that are described herein.

We thank and acknowledge our collaborators, and GMDSI project funders, for making these reports possible.

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GLOSSARY

Anisotropy

A condition whereby the properties of a system (such as hydraulic conductivity) are likely to show greater continuity in one direction than in another. At a smaller scale it describes a medium whose properties depend on direction.

Bayesian analysis

Methods that implement history-matching according to Bayes equation. These methods support calculation of the posterior probability distribution of one or many random variables from their prior probability distributions and a so-called “likelihood function” – a function that increases with goodness of model-to-measurement fit.

Boundary condition

The conditions within, or at the edge of, a model domain that allow water or solutes to enter or leave a simulated system.

Boundary conductance

The constant of proportionality that governs the rate of water movement across a model boundary in response to a head gradient imposed across it.

Capture zone

The three-dimensional volumetric portion of a groundwater flow field that discharges water to a well.

Connected linear network (CLN) package

This package is supported by the MODFLOW-USG simulator. Water flows through a series of one-dimensional features, each of which can be linked to another such feature, or to a cell within a two or three-dimensional groundwater model domain.

Contributing area

The two-dimensional areal extent of that portion of a capture zone that intersects the water table and surface water features where water entering the groundwater flow system is discharged by a well. (This is also referred to as the *area contributing recharge.*)

Covariance matrix

A matrix is a two-dimensional array of numbers. A covariance matrix is a matrix that specifies the statistical properties of a collection of random variables - that is, the statistical properties of a random vector. The diagonal elements of a covariance matrix record the variances (i.e. squares of standard deviations) of individual variables. Off-diagonal matrix elements record covariances between pairs of variables. The term “covariance” refers to the degree of statistical inter-relatedness between a pair of random variables.

Ensemble

A collection of realisations of random parameters.

Drain (DRN) package

A one-way Cauchy boundary condition implemented by MODFLOW. Water can flow out of a model domain, but cannot enter a model domain through a DRN boundary condition.

Evapotranspiration (EVT) package

MODFLOW's simulation of plant evapotranspiration and direct evaporation from a groundwater system. The extraction rate increases, up to a user-supplied maximum rate, as the water table approaches a user-prescribed elevation from below. If the water table falls below a user-specified extinction depth, evapotranspiration ceases.

General head boundary (GHB) package

This is MODFLOW parlance for a Cauchy boundary condition. Water flows into or out of a model domain in proportion to the difference between the head ascribed to the boundary and that calculated for neighbouring cells. The rate of water movement through the boundary in response to this head differential is governed by the conductance assigned to the boundary.

Hydraulic conductivity

The greater is the hydraulic conductivity of a porous medium, the greater is the amount of water that can flow through that medium in response to a head gradient.

Jacobian matrix

A matrix of partial derivatives (i.e. sensitivities) of model outputs (generally those that are matched with field measurements) with respect to model parameters.

Matrix

A two-dimensional array of numbers indexed by row and column.

MODFLOW

A family of public-domain, finite-difference groundwater models developed by the United States Geological Survey (USGS).

MODFLOW-USG

A version of MODFLOW which employs an unstructured grid. This was developed by Sorab Panday in conjunction with the United States Geological Survey (USGS).

MODFLOW package

An item of simulation functionality that describes one aspect of the operation of a groundwater system, for example recharge or a boundary condition. The word "package" describes the computer code that implements this functionality, as well as its input and output file protocols.

MODPATH

A family of MODFLOW suite postprocessors that undertake particle-tracking in MODFLOW-calculated flow fields.

Mod-PATH3DU

A particle tracking program that can accommodate unstructured grids. It can evaluate particle tracks in flow fields computed by programs of the MODFLOW suite, and by MODFLOW-USG.

Null space

In the parameter estimation context, this refers to combinations of parameters that have no effect on model outputs that are matched to field observations. These combinations of parameters are thus inestimable through the history-matching process.

Objective function

A measure of model-to-measurement misfit whose value is lowered as the fit between model outputs and field measurements improves. In many parameter estimation contexts the objective function is calculated as the sum of squared weighted residuals.

Parameter

In its most general sense, this is any model input that is adjusted in order to promote a better fit between model outputs and corresponding field measurements. Often, but not always, these inputs represent physical or chemical properties of the system that a model simulates. However there is no reason why they cannot also represent water or contaminant source/sink strengths and locations.

Phreatic surface

The water table.

Pilot point

A type of spatial parameterisation device. A modeller, or a model-driver package such as PEST or PEST++, assigns values to a set of points which are distributed in two- or three-dimensional space. A model pre-processor then undertakes spatial interpolation from these points to cells comprising the model grid or mesh. This allows parameter estimation software to ascribe hydraulic property values to a model on a pilot-point-by-pilot-point basis, while a model can accept these values on a model-cell-by-model-cell basis. The number of pilot points used to parameterise a model is generally far fewer than the number of model cells.

Prior probability

The pre-history-matching probability distribution of random variables (model parameters in the present context). Prior probability distributions are informed by expert knowledge, as well as by data gathered during site characterisation.

Posterior probability

The post-history-matching probability distribution of random variables (model parameters in the present context). These probability distributions are informed by expert knowledge, site characterisation studies, and measurements of the historical behaviour of a system.

Probability density function

A function that describes how likely it is that a random variable adopts different ranges of values.

Probability distribution

This term is often used interchangeably with “probability density function”.

Quadtree mesh refinement

This term refers to a means of creating fine rectilinear model cells from coarse rectilinear model cells by dividing them into four. Each of the subdivided cells can then be further subdivided into another four cells. However it is a design specification of a quadtree-refined grid that no cell within the domain of a model be connected to more than two neighbouring cells along any one of its edges.

Realisation

A random set of parameters.

Regularisation

The means through which a unique solution is sought to an ill-posed inverse problem. Regularisation methodologies fall into three broad categories, namely manual, Tikhonov and singular value decomposition.

Residual

The difference between a model output and a corresponding field measurement.

River (RIV) package

A MODFLOW package which provides basic simulation of the interaction between groundwater and a surface water body. Flow between the two regimes is driven by the head difference between them. Through definition of the elevation of the bottom of the river, the driving head difference can be limited.

Singular value decomposition (SVD)

A matrix operation that creates orthogonal sets of vectors that span the input and output spaces of a matrix. When undertaken on a Jacobian matrix, SVD can subdivide parameter space into complementary, orthogonal subspaces; these are often referred to as the solution and null subspaces. Each of these subspaces is spanned by a set of orthogonal vectors. The null space of a Jacobian matrix is composed of combinations of parameters that have no effect on model outputs that are used in its calibration, and hence are inestimable.

Solution space

The orthogonal complement of the null space. This is defined by undertaking singular value decomposition of a Jacobian matrix.

Specific storage

The amount of water that is stored elastically in a cubic metre of porous medium when the head of water in which that medium is immersed rises by 1 metre.

Specific yield

The amount of accessible water that is stored in the pores of a porous medium per volume of that medium.

Stochastic variable

A stochastic variable is a random variable.

Stress

This term generally refers to those aspects of a groundwater model that cause water to move. They generally pertain to boundary conditions. User-specified heads along one side of a model domain, extraction from a well, and pervasive groundwater recharge, are all examples of groundwater stresses.

Stress period

The MODFLOW family of models employs this terminology to describe each member of a series of contiguous time intervals that collectively comprise the simulation time of a model.

Tikhonov regularisation

An ill-posed inverse problem achieves uniqueness by finding the set of parameters that departs least from a user-specified parameter condition, often one of parameter equality and hence spatial homogeneity.

Time-variant specified head (CHD) package

This is a Dirichlet (i.e. “fixed head”) boundary condition implemented by MODFLOW in which the head can vary with time on a stress-period-by-stress-period basis.

Vector

A collection of numbers arranged in a column and indexed by their position in the column.

Well (WEL) package

A MODFLOW package that simulates withdrawal of water from a groundwater system.

EXECUTIVE SUMMARY

Identification of the locations of present-day or historical contaminant releases provides multiple layers of difficulty. Not one, but two inverse problems must be solved. The first is that of inferring the source (or sources) of contaminants whose presence has been detected in the groundwater system. The second is that of inferring the groundwater flow field that has transported these contaminants to wells in which they have been detected. This flow field depends on subsurface hydraulic properties, as well as on groundwater recharge, and on interaction of groundwater with surface water bodies. Details of all of these are generally poorly known. These must therefore be inferred from the same data as that from which contaminant source locations must be inferred.

The problem is made more difficult by the nature of the data from which these inferences must be drawn. Borehole measurements of contaminant concentration are “noisy”; they are strongly affected by local conditions; they can be highly depth-dependent. Use of these data in inverse problem-solving is further compounded by the approximate nature of solute transport simulation. These approximations include a tendency to “blur” simulated concentrations through numerical dispersion, and through the necessity to simulate hydrodynamic dispersion as a surrogate for the effects of local-scale heterogeneity which are beyond the capacity of a numerical model to either represent or simulate. The use of complex, advection-dispersion based simulators in inverse problem-solving is further compounded by their slow execution speed, and by their sometimes problematical numerical behaviour.

While these difficulties should be recognized, the imperative to process site contaminant data in order to draw inferences about contaminant source locations cannot be ignored. However, methodologies for processing of these data should accommodate inverse problem nonuniqueness, and hence the need to present outcomes of data processing in probabilistic ways that inform decision-makers of what can be known, and of what cannot be known. They should also recognise the difficulties associated with attempts to access limited information from messy data, and the requirement for speed of numerical simulation so that obstacles to probabilistic, model-based assimilation of site data can be reduced.

We present such a method in this GMDSI worked example report. It is based on innovative use of particle-tracking instead of advection-dispersion modelling. Simulation is therefore rapid; model runs can be repeated many times using different stochastic parameter fields. This enables data assimilation; it also enables probabilistic representation of data assimilation outcomes. The methodology recognizes that borehole measurements of contaminant concentration often provide little information beyond that which identifies whether a contaminant plume exists at a particular location or not. However it also recognizes that this information is worthy of inclusion in the two-tiered inverse problem that the search for contaminant sources poses, for this information potentially possesses the capacity to reduce uncertainties associated with inferences of subsurface properties, and with inferences of contaminant source location.

We apply this method to data that was gathered in Pavia, an industrial city in the north of Italy. Data and site information were kindly provided by the Provincial Administration of Pavia. We use MODFLOW 6 to simulate groundwater flow, MODPATH 7 to calculate particle tracks, PEST_HP for model calibration and PESTPP-IES for probabilistic inversion. We follow the Bayesian precept that facets of the groundwater system which are poorly known should be represented probabilistically. This allows the repercussions of our incomplete knowledge of subsurface properties and processes to be reflected in parameter and predictive uncertainty, rather than in unquantifiable predictive bias. At the same time, we constrain predictive uncertainties through formulation of an inverse problem that is based on borehole head

measurements, and on binary-classified borehole contaminant concentration measurements that identify whether a borehole is within or without a contaminant plume at a particular point in time.

Outcomes of our analysis are encapsulated in two probability maps. The first of these maps depicts the probability that if a source exists at a particular location, then contaminants that are released from that source will go undetected by the present groundwater monitoring network. The second map depicts the probability that a contaminant source does not exist at a particular location. Taken together, these two maps say as much as can be said about contaminant source location, given site data that is considered in this report. (These data pre-date those which have since been collected at Pavia following initiation of remediation activities).

With the ability to quantify predictive uncertainty comes the ability to quantify reduction in predictive uncertainty. Uncertainty is reduced through acquisition of further data. We extend our methodology to quantify data worth. We demonstrate how probability maps based on the present observation network may be enhanced by inclusion of measured contaminant concentrations in boreholes that have not yet been drilled. The advantages of drilling a new hole at one potential location over drilling a new hole at another potential location can thereby be assessed.

CONTENTS

1. INTRODUCTION

1.1 General

In this short worked example report, we discuss an issue that groundwater modelling is often asked to address. The issue is that of identifying potential sources of groundwater contamination.

Much has been written on this subject. A recent paper by Gómez-Hernández and Xu (2021) provides a thorough and easy-to-read review. Their review summarises the application of latest modelling technology to this difficult problem. They point out that most cases that are documented in the literature are synthetic rather than real. This is partly due to the fact that real-world groundwater contamination problems tend to be politically sensitive, and that their associated datasets are often closely guarded secrets. It is also partly due to the fact that contaminant source detection is an inherently difficult problem.

Finding the source of a contaminant requires solution of an inverse problem. The location, and sometimes the timing, of a contaminant source must be back-calculated from measurements of contaminant concentration that were made in wells. Obviously, these wells must lie downstream of the contaminant source. Or, to put it another way, a crude solution of the inverse problem of source detection is that the source of a contaminant must lie upstream of wells in which a contaminant has been detected.

Unfortunately, the notion of “upstream” leaves a lot of room for error. Flow of groundwater is affected by many factors, including hydraulic property heterogeneity, groundwater extraction, recharge patterns and interaction of shallow groundwater with surface water bodies. Furthermore, it is not uncommon for a number of possible contaminant sources to exist in the same neighbourhood. Solution of the inverse problem that seeks these sources should attempt to resolve them spatially. Alternatively, it may demonstrate that this is not possible; in this case it should identify how the current disposition of monitoring wells should be expanded in order to provide the desired spatial resolution of contaminant source inference.

The subsurface is heterogeneous. The distribution of hydraulic properties within it is complex. This distribution must be inferred from a handful of direct measurements of these properties (which are often at the wrong scale), and/or back-calculated from borehole measurements of groundwater head and contaminant concentration. This presents those who seek contaminant sources with two inverse problems, namely that of back-calculating the distribution of subsurface properties, as well as that of back-calculating contaminant source locations. To make matters worse, in urban and industrial areas, recharge is often only vaguely known, so this too must be back calculated, along with conditions that prevail at the interface between the groundwater system and permanent or transient surface water bodies.

Solution of this complex, high-dimensional inverse problem is obviously nonunique. Inferences of contaminant source location can only therefore be probabilistic. Posing of the problem requires a high level of sophistication.

The inverse problem is made even more difficult by the nature of the data that it must process. The concentration of a contaminant at a particular measurement location and depth is affected not just by the presence of one or more upstream sources. It is also affected by local nuances of the subsurface in the vicinity of the measurement well. These can include the spatial disposition of sand and clay layers, as well as the intricate patterns of weathering and fracturing that determine the torturous paths that are taken by contaminants in the shallow subsurface. In geologically heterogeneous settings, the information content of subsurface measurements of contaminant concentration may therefore be limited to that of indicating whether or not a contaminant plume exists at that location.

Another set of problems accompanies the use of current contaminant transport simulation technology. Numerical solution of the advection-dispersion equation requires use of a model whose execution time is long, and whose numerical health is often delicate. Problems with execution speed are exacerbated if a model is endowed with a small cell size and with many layers in order to reduce the propensity for numerical dispersion, and/or to provide a basis for stochastic representation of fine-scale subsurface heterogeneity. Solution of a complex, stochastic inverse problem requires that a model be run thousands of times using complex parameter fields. Long run times and numerical instability may make this impossible.

Particle-tracking presents an alternative means of simulating advective contaminant movement. It is computationally fast and numerically stable. However, execution can become slow where particles number in the tens of thousands (as they do in the work described herein). Nevertheless the unwavering numerical stability of particle track calculations can facilitate solution of complex probabilistic inverse problems that would otherwise be challenged by reliance on repeated solution of the advection-dispersion equation.

In this report we demonstrate a new methodology for contaminant source assessment that relies on heavy-duty particle tracking. We show how particles can be used not just for probabilistic location of contaminant sources, but also for reducing the uncertainties that are associated with estimation of contaminant source locations. We also demonstrate how particles can provide a powerful, yet numerically cheap, basis for model history-matching. It is through history-matching that the information content of borehole contaminant measurements can be used to reduce the uncertainties of inferred contaminant source locations, and of the hydraulic properties of the medium through which contaminants are transported prior to being detected.

1.2 Modelling Philosophy

The approach to groundwater modelling that is demonstrated by this worked example is similar to that which is demonstrated by other GMDSI worked examples. We do not see ourselves in particular, nor human beings in general, as being capable of simulating subsurface processes very well. Nor do we aspire to do so. What we aspire to do is to process environmental data in ways that can help someone to make a decision. This requires that the decision-maker be fully acquainted with the risks that accompany its making. Quantification of the uncertainties of decision-critical model predictions therefore becomes a necessity, as does reduction of these uncertainties where data allow it.

Doherty and Moore (2021) explain that quantification and reduction of model predictive uncertainty generally (but not always) requires use of a structurally simple but parametrically complex model. This is because structural complexity runs the risk of hardwiring disinformation into model-based data processing. This can induce predictive bias. Doherty and Moore also explain that model parameters are carriers of information; they can do this because (by definition) they are adjustable. This allows them to “wiggle” in response to information paucity, and for their “wiggle room” to be constrained when informed by field measurements of system states and fluxes through history-matching.

To be sure, excessive structural simplicity may require that parameters adopt roles that compensate for model structural imperfections. This may distort the information that they carry. Part of the role of decision-support model design is to reduce the propensity for this to occur. Conceptually, the predictive ramifications of parameter information distortion can be included in predictive confidence intervals. Meanwhile, through careful, prediction-tuned model design, reductions in predictive uncertainty accrued through data assimilation can more than compensate for increases in predictive uncertainty incurred by the (hopefully) small degree of information distortion that enables data assimilation to occur.

The pursuit of probabilistic model outcomes allows the uncertainties of decision-critical model predictions to be explored. With quantification of predictive uncertainty comes the ability to assess the capacity for new data to reduce predictive uncertainty. In this report we show how the methodology that we describe herein is readily adapted to the important task of improving and optimizing the design of a monitoring network.

The procedure for model-based processing of contaminant measurements that is described in this report is relatively easy to employ at any field site that is the focus of contaminant source investigations. Software has been added to the PEST Groundwater Utility Suite that is able to undertake the necessary post-processing of model-calculated particle tracks. Appendix A lists programs that have been recently added to that suite for this purpose.

1.3 What Lies Ahead

This short report is organised as follows.

Section 2 describes the site that is the focus of the current investigation. Section 3 describes the methodology that is used for particle-based data assimilation and contaminant source probability assessment. Section 4 describes model design, construction and history-matching. Section 5 describes model deployment for contaminant source assessment; it also discusses how modelling can be used to optimise expansion of the current modelling network. Section 6 concludes the report.

2. THE SITE

2.1 General

Pavia is situated in the north of Italy, about 40 km south of Milan. In common with many industrial areas throughout the world, PCE, TCE and related compounds have been detected in groundwater. Detection of these compounds in Pavia groundwater precipitated a series of investigations whose purpose was to identify the disposition of contaminant plumes, and to link these plumes to sources. Of particular interest are a number of abandoned industrial sites that are situated not too far from the Pavia city centre. This is a densely populated area that hosts a rich spectrum of commercial, artisanal and industrial activities.

2.2 Disclaimer

We provide only a brief description of the study site, and of measurements that have emerged from characterisation of that site. We provide only enough information for a reader to gain an understanding of site conditions (which are not atypical of those that prevail at many contaminated sites), and to understand the approach to model-based processing of site data that is documented in ensuing sections of this report. We do not itemize the names and concentrations of all detected contaminants. Furthermore, we restrict our processing of site data to that which was gathered prior to 2017.

Data that expose groundwater contamination are always sensitive. We are deeply grateful to the Provincial Administration of Pavia to have given us access to data that are discussed herein. The focus of this report is demonstration of a methodology that can be readily deployed to process data such as these. It is not to draw any conclusions pertaining to contaminant sources in Pavia. That task belongs to others.

Note that in 2017, remediation and containment actions were activated at the site. Additional monitoring points were also established. These are not discussed in this report.

2.3 Topographic Setting

The area of interest, which includes the city of Pavia, slopes gently to the south towards the Ticino River. It lies between 75 and 85 metres above mean sea level. The Ticino River is incised 10 m to 15 m into surrounding plainlands. See Figure 2.1.

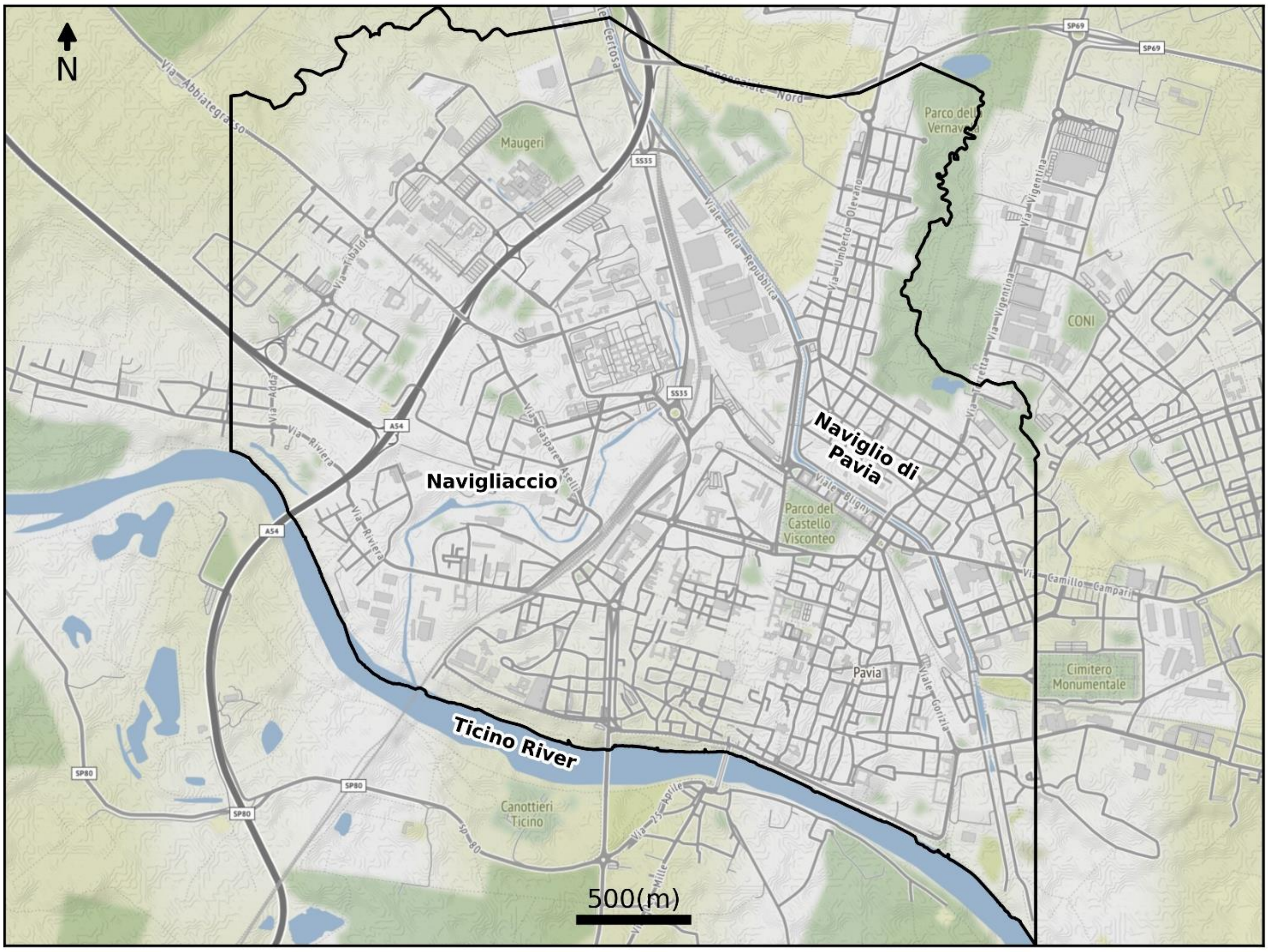

Figure 2.1. Map of the study area.

Two canals flow through the area of interest. These are the Naviglio di Pavia and Navigliaccio Canals. Both of these canals are in hydraulic connection with the groundwater system. The Navigliaccio Canal is of particular relevance to the present study as many of the observation wells in which contaminant concentration and head measurements have been made are situated close to it. The Navigliaccio Canal is thought to contribute water to the groundwater system over part of its length, and to receive groundwater in other places.

2.4 Hydrogeology

Pavia is situated within the broad alluvial plain of the River Po. The floodplain is characterised by gravels, sands and silts that were deposited from late Pliestocene to recent times. In places, these sediments are eroded to form river terraces which provide local topographic relief.

Three separate aquifers are recognized in the vicinity of Pavia. A thin, perched aquifer with a coarse sandy matrix is found under parts of the study area; this is referred to as the FFS aquifer in consultants' reports. Where it exists, the base of the FFS aquifer is generally within 10 m of the land surface. It is discontinuous, and is thought to be responsible for little, if any, lateral movement of contaminants. Hydrogeologically, its principal role is to delay recharge to the unconfined aquifer which lies beneath it.

The unconfined aquifer that enables contaminant movement is comprised of fine to medium sands with some gravel. It extends to a depth of about 35 metres below the ground surface. This is referred to as the FFB aquifer. This aquifer is thought to be heterogeneous and locally compartmentalized by thick clay lenses. The FFB aquifer is in direct contact with the Ticino River, the Naviglio di Pavia Canal and parts of the Navigliaccio Canal. Hydraulic property heterogeneity within this aquifer is intensified by the presence of a paleochannel near parts of the Navigliaccio Canal, this being an outcome of historical rerouting of the canal. Pumping tests reveal vertically-averaged hydraulic conductivities of between 8 m/d and 40 m/d.

Other aquifers underly the FFB aquifer. However, they are separated from it by impermeable clay layers. At the present time, water within these aquifers is considered to be hydraulically isolated from those that saturate the FFB aquifer, at least in the vicinity of Pavia. The aquifer immediately below the FFB is therefore thought to play no role in local contaminant movement.

2.5 Recharge

In common with all urban areas, recharge under Pavia is heterogeneous. Higher rates of recharge may occur where there are holes in the unconfined FFS aquifer, and through outcropping sediments of the Navigliaccio Canal paleochannel. For convenience, previous studies have assumed a spatially averaged value of about 200 mm/year.

The FFB aquifer may be recharged locally by seepage from canals. It loses water to canals in other places. As is discussed in Section 4 of this document, interaction of the groundwater system with the surface water system is simulated using appropriate boundary conditions.

2.6 The Monitoring Network

Contaminants were probably introduced to the Pavia alluvial system by spills and leakages that occurred in a number of factories, all of which are now closed. Contamination of the aquifer is thought to have commenced between 50 and 60 years ago.

Intense, piezometric and chemical sampling of the FFB aquifer began in 2004, and has continued up until the present day. In the present study we consider measurements that were made during and prior to 2016. Shortly after this date, a system of extraction wells was installed near the Navigliaccio Canal in order to withdraw contaminant from the aquifer. Prior to that date, the piezometric surface in the study area has varied little over time; in modelling that is documented later in this report, steady state conditions are assumed to prevail.

Observation wells have been variously sampled for PCE (perchloroethylene), TCE (trichloroethane), TCM (chloroform or trichloromethane), 1,1-dichloroethylene and 1,1-dichloropropanol. The most consistent sampling has been for PCE, so we focus on this contaminant in the present study. PCE is used for degreasing of metal parts, dry cleaning, production of CFC substitutes, and processing in the textile sector. With loss of chlorine, PCE degrades to TCE, 1,2-dicholoroethylene and other daughter products.

As is usual for chemical sampling of observation wells, variability of contaminant concentration with sampling depth, and with sampling location, is high. This is not unexpected as the vertical concentration profile of a contaminant is likely to be affected by vertical variations of aquifer permeability, by details of lateral groundwater movement through a horizontally-heterogeneous subsurface, by local recharge, and by decay and dispersion. Nevertheless, investigations have revealed the existence of what are thought to be a number of discrete plumes, revealing the possibility of a number of discrete contaminant sources.

In the study that is reported herein, we do not directly process measured concentrations because these are almost impossible to reproduce using a numerical model. Instead, we use PCE measurements to divide observation wells into two categories. The first category is composed of wells in which contamination has been detected, while the second category is composed of wells in which contamination has not been detected. For data-processing purposes, we adopt a PCE plume detection threshold of 1.1 µg/l. Detect and nondetect wells are plotted in Figure 2.2. This figure also depicts wells in which piezometric head measurements were made.

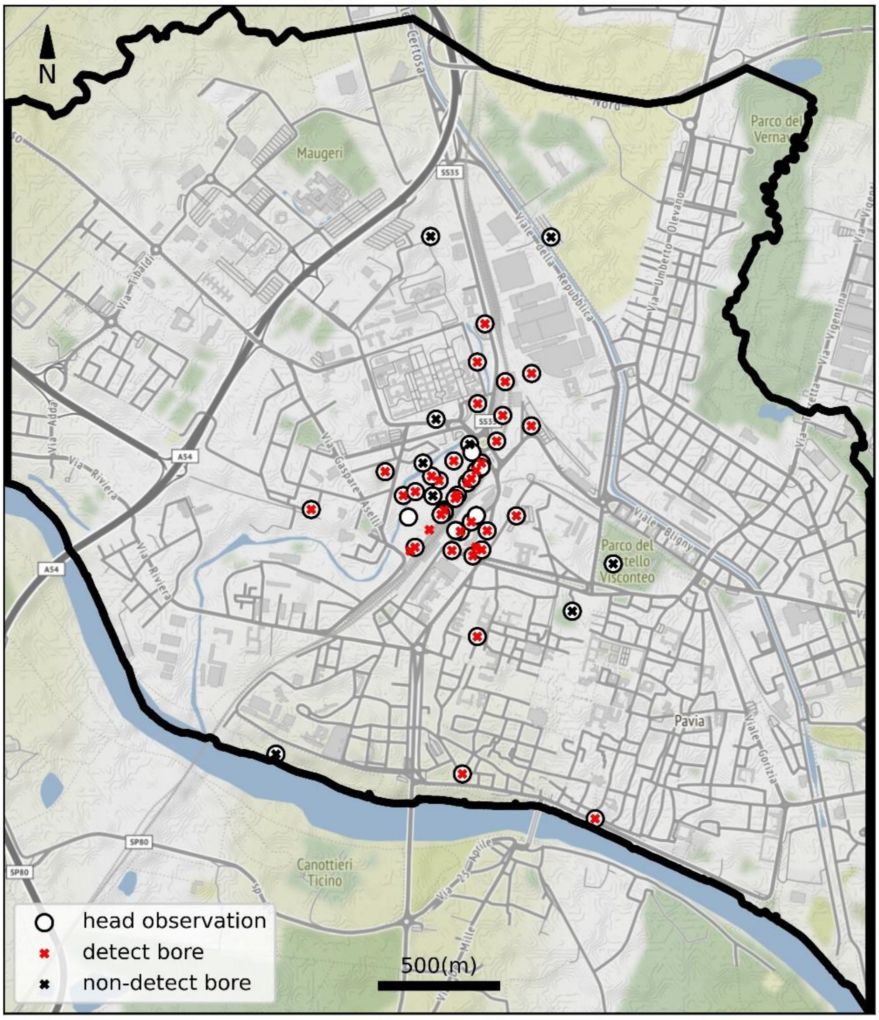

Figure 2.2 Observation wells.

3. PROCESSING OF CONTAMINANT DATA

3.1 History-Matching against Concentration Measurements

Models that are used to support the making of decisions require history-matching. Rarely does this result in estimation of a unique parameter field. However it forms a basis for analyses wherein the probability distributions of predictions of interest can be quantified and constrained. Predictive uncertainty reduction is accrued though insistence that any parameter field that is used by a model to make a prediction of management interest must also allow the model to reproduce observations of the historical behaviour of the system that it simulates, to within limits set by measurement noise. This affects the character and spatial variability of parameter fields that the model can use when making a prediction.

Obviously, if the purpose of a model is to infer contaminant source locations from borehole measurements of groundwater chemistry, then it must reproduce the contaminated status of the groundwater system at wells that intersect a contaminant plume. However, this is not the only reason why a model which is used for this purpose must be capable of reproducing these statuses. Moore and Doherty (2005) show that the information content of head measurements with respect to predictions of contaminant movement is low. Hence history-matching against heads alone may do little to reduce the uncertainties of contaminant fate and source predictions. On the other hand, because solute transport is so sensitive to subsurface heterogeneity, measurements of contaminant concentration can provide information about the properties and character of subsurface heterogeneity that head measurements cannot.

Solute concentrations can be calculated using an advection-dispersion model. Models such as FEFLOW, MODFLOW/MT3DMS, MODFLOW-USG and MODFLOW 6 are commonly used to calculate the spatial distribution of solute concentrations within an aquifer that arise from a known solute source. However, history-matching of concentrations calculated by these models against borehole-measured concentrations is beset with problems. As discussed above, the measured concentration of a contaminant at any point in the subsurface is profoundly affected by local conditions – conditions that prevail at too fine a scale for inclusion in an advection-dispersion model. In everyday modelling practice, this is recognized by inclusion of hydrodynamic dispersion as an agent for contaminant migration and spreading in lieu of direct representation of small-scale hydraulic property variability. If the latter were, in fact, represented in a model, it would require stochastic representation, for while its existence may be known, its details cannot be known.

However hydrodynamic dispersion provides only an abstract representation of far more complex processes. In general, "simulation" of hydrodynamic dispersion does not improve a model's ability to reproduce field-measured concentrations, especially in highly heterogeneous aquifers such as those that prevail under Pavia. A modeller must therefore tolerate a low level of model-to-measurement fit, while allowing hydrodynamic dispersion to "smudge out" contaminant plume boundaries, as he/she attempts to reproduce measured concentrations using an advection-dispersion model. This approach to history-matching of contaminant data runs the risk of devaluing the information content of these data, especially where contaminant plume boundaries appear to be sharp, as is the case at Pavia.

History-matching of contaminant concentrations that are calculated by an advection-dispersion model encounters other difficulties. Use of such a model implies that a solute source is known. However the object of modelling may be to locate the source. Conceptually, this can be achieved by running the advection-dispersion process backwards through a flow field computed by a groundwater model; see, for example, Aberladom and Nowak (2018), Frind and Molson (2018) and Neupauer and Wilson (2002). Unfortunately, however, simulators which do this are not available to the public. Furthermore, use of this strategy does not take advantage of the data assimilation and uncertainty-reduction opportunities that history-matching against contaminant measurements affords.

Adding to these problems is the fact that advection-dispersion simulators tend to run slowly. They require many layers and small cell sizes to mitigate the effects of numerical dispersion. When endowed with stochastic parameter fields (as is required for probabilistic exploration of contaminant source location), their numerical stability may suffer.

3.2 Contaminant Detection as a History-Matching Target

Because of problems such as those outlined above that afflict history-matching against measurements of solute concentration, we adopt a different strategy. For modelling that is documented herein, this strategy is made easier by the fact that the groundwater flow field is close to steady state. However, as the following description shows, our methodology does not rely on the presumption of steady state conditions. Nevertheless, the presumption of steady state conditions does have the benefit that a single contaminant-related observation can be ascribed to each measurement well. This is the observation that a contaminant was, or was not, detected in that well. (A more complex implementation of the methodology discussed herein would require that a time be associated with each such detect/nondetect observation.)

Each Pavia observation well that was sampled for the presence of groundwater contamination is therefore endowed with a binary status. The well is classified as either a “detect well” or a “nondetect well”. It is awarded the former status if the PCE concentration has ever exceeded 1.1 µg/l. Because of the messy nature of borehole solute concentration measurements, this binary classification of observation well status may, in fact, capture most of the information that contaminant datasets can offer.

A potential problem with binary observations is lack of differentiability with respect to model parameters. Differentiability is essential for use of observations in highly-parameterized history-matching. This problem is overcome in ways that we now describe.

3.3 Particles

As is discussed in Section 4 of this document, a groundwater model was built in order to seek contaminant sources. Its domain encompasses the town of Pavia, including all monitoring wells and all possible locations of contaminant leakage and spillage. Steady state conditions are assumed to prevail.

Particles are released throughout the domain of this model. The methodology that we now describe can accommodate high particle densities – up to one particle per model cell throughout the entirety of the model domain. If this number of particles is considered excessive, then their release can be confined to areas where contaminant sources are likely to exist.

In the present study, particles are allowed to advect for up to 50 years. This corresponds to the time over which contaminant is thought to have leaked into the Pavia groundwater system.

3.4 Particle Status

Figure 3.1 schematically depicts the path of a particle. Its journey begins in the cell in which it is released; entrained by the groundwater flow field, it winds its way through the model domain until it encounters a sink, or until its allocated simulation time has expired.

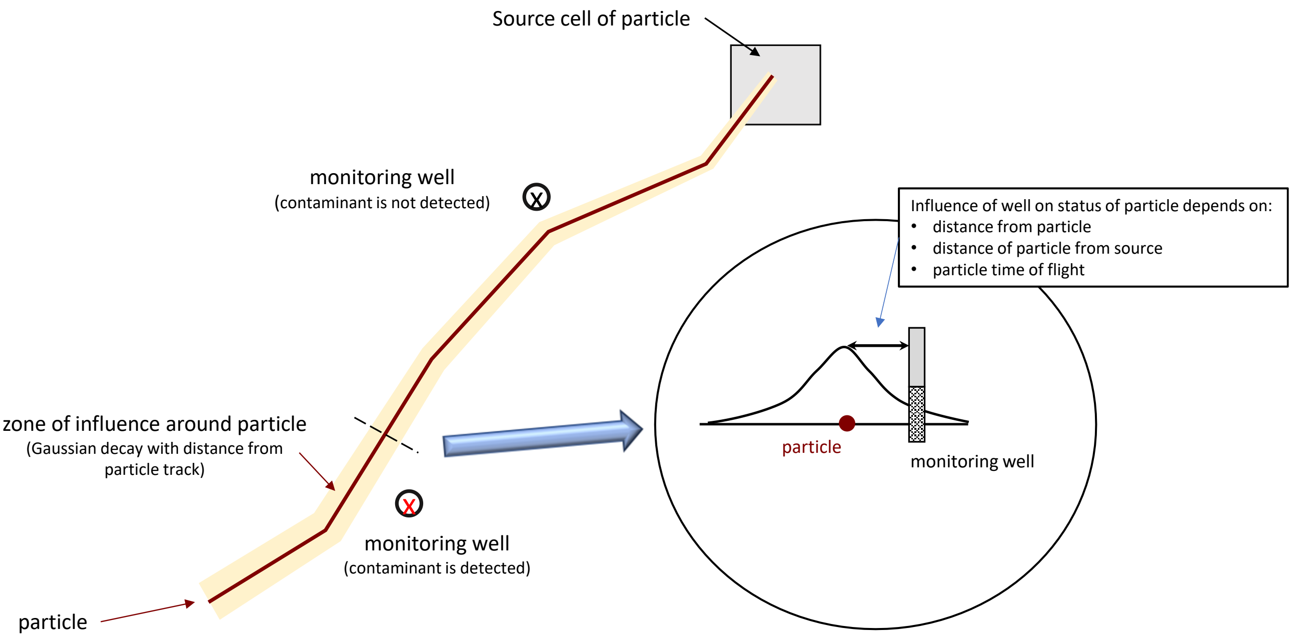

Figure 3.1. Particle path and surrounding field of influence.

We assign an "influence function" to the particle. This function decays with distance from its trajectory in the same way that a Gaussian bell curve decays with distance from its peak. The maximum value of this influence function is 1.0. The dependence of its value *w* on distance from the particle trajectory is described by the following equation:

$$w = exp\left[-\left(\frac{d}{a}\right)^2\right] \qquad (3.1)$$

In equation 3.1, *d* is the distance from the particle trajectory while *a* is the distance at which the value of *w* has fallen to about 0.37. *a* is calculated using the following equations:

$$a = a_0 + (a_1 - a_0)\frac{s}{s_1} \qquad \text{if } s \le s_1 \qquad (3.2a)$$

$$a = a_1 + m(s - s_1) \qquad \text{if } s > s_1 \qquad (3.2b)$$

In the above equations a_0, a_1, *m* and s_1 are provided by the modeller. The variable *s* denotes the total distance travelled by the particle to the point where *w* is evaluated. The influence distance of a particle can thus increase with its travel distance. See Figure 3.2.

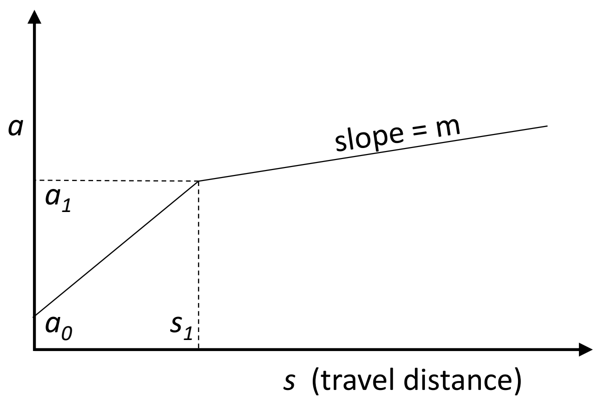

Figure 3.2. The influence distance of a particle can increase as its travel distance increases.

The notion of a Gaussian influence function centred on an advectively-transported particle resembles the influence of diffusion on solute concentration as calculated using analytical solutions of the advection-dispersion equation.

Now suppose that the particle passes close to an observation well in which contaminant has been detected. Equation 3.1 can be used to award the particle a “detect status”. In awarding it this status, *d* of equation 3.1 is the distance of closest approach of the particle to the well. Utility software supplied with the PEST Groundwater Utility Suite allows the influence of a detect well on a particle’s detect status to decay with particle time of flight; this accommodates contaminant degradation during transport. This option is not implemented in the present study.

We denote the detect status of a particle as *D*.

In a similar manner to that in which a particle can be awarded a detect status if it passes close to a detect well, it can also be awarded a nondetect status if it passes close to an observation well in which contaminant is not detected (i.e. a nondetect well). Let us denote its nondetect status as *N*.

A particle can also be awarded an inconsistency status I. This is calculated as:

$$I = [DN]^{\alpha} \tag{3.3}$$

where α is supplied by the modeller. (We use 1.0 in the present case.)

It is important to note that a particle’s detect/nondetect/inconsistency status is a continuous function of distance *d* between the track of a particle and the location of a nearby observation well. At the same time, coordinates of a particle’s track are continuous functions of model parameter values, provided that these values do not vary too much. (If a parameter such as hydraulic conductivity varies too much, a particle may embark on a different course altogether; it may decide to go around a hydraulic conductivity obstacle instead of going through it). Hence “observations” of particle status are, conceptually at least, useable components of an objective function whose minimization can yield a parameter field of minimum error variance; this occurs when a model undergoes calibration. Alternatively, this objective function can be used to constrain stochastic parameter fields in probabilistic history-matching. We demonstrate both of these in the next section of this document.

Figure 3.3 illustrates the inconsistency status of a particle for three dispositions of observation wells around a particle track.

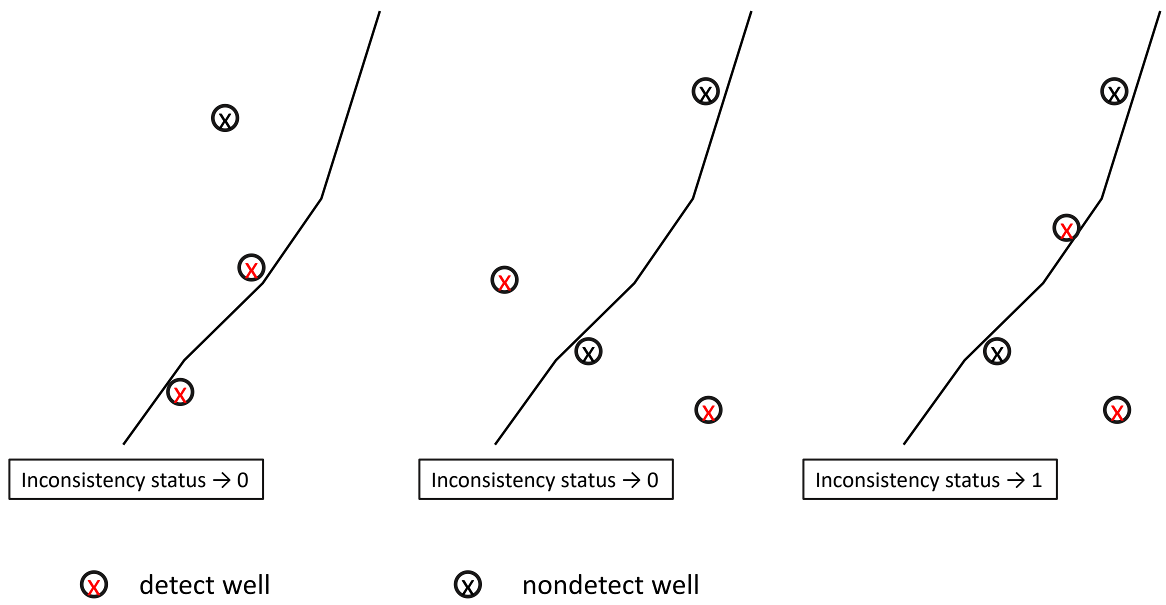

Figure 3.3. Examples of particle inconsistency status.

Because no more than one particle is allowed to originate in each model cell, the model cell in which a particular particle's journey commences can inherit that particle's detect/nondetect/inconsistency status. This allows the cell's status as a possible contaminant source to be examined.

Values of 6.25 m, 6.25 m, 500 m and 0 for a_0, a_1, s_1 and m are employed in Pavia modelling. The resulting a value is commensurate with the width of Pavia model cells (see the next section). Its small value, and use of an m value of zero, implies limited hydrodynamic dispersion. This accommodates the fact that some Pavia wells that detect a contaminant are not too far from wells in which contaminant was not detected. It also accommodates the fact that dispersivity can often be assigned a relatively low value when hydraulic property heterogeneity is explicitly represented in a model, rather than implied by hydrodynamic dispersion. Spatial hydraulic property heterogeneity is, in fact, explicitly represented in the Pavia model through the use of history-match-constrained stochastic parameter ensembles based on a high spatial density of pilot points.

3.5 More on History-Matching

Measured heads comprise part of the history-matching dataset of most groundwater models. This applies to the Pavia model. As will be described in the next section, the history-matching dataset also includes observations that ensure integrity of model-calculated boundary heads, for these are parameterized, and hence adjustable.

It is stated above that solute concentration measurements are rich in information on subsurface hydraulic property heterogeneity – more so than measurements of piezometric head. However this information is degraded by "noise" arising from sensitivity to local hydrogeological conditions, and by "blurring" of concentrations that are calculated by an advection-dispersion model.

Because the Pavia model does not calculate solute concentrations, measured contaminant concentrations cannot be used directly in the history-matching process. However, as is now described, particle-based surrogates for contaminant concentration can be used in the history-matching process. The high information content of contaminant observations can therefore constrain model parameters, and hence reduce the uncertainties of at least some contaminant-related model predictions.

The track of a particle depends on the groundwater flow field. This, in turn, depends on the model's parameter field. For a given parameter field, each particle is endowed with a detect status, a nondetect status and an inconsistency status. Where particle placement is dense and pervasive then thousands, or even tens of thousands, of particles may traverse a model domain. Those that do not pass near either a detect or a nondetect well are awarded a detect status of zero, a nondetect status of zero and an inconsistency status of zero. Those that pass near a detect well are awarded a non-zero detect status, while those that pass near a nondetect well are awarded a nonzero nondetect status. If a particle passes close to both a detect well and a nondetect well, then it is awarded a non-zero inconsistency status. This implies that the particle carries a quantum of contaminant mass; at the same time it implies that the particle does not carry a quantum of contaminant mass. Obviously, this is impossible. Hence a parameter field which allows this to occur is also impossible.

To preclude history-match emergence of an impossible parameter field, one observation per particle is introduced to the history-matching dataset. This observation states that the inconsistency status of the particle is zero. Differences between observed and model-calculated particle inconsistency statuses are thereby included in the history-matching objective function. The objective function is lowered when such inconsistencies are prevented. This induces PEST/PEST++ to avoid parameter fields which promulgate particle inconsistency.

Through this mechanism, information that is contained in measurements of groundwater contaminant concentration are transferred to parameters, and hence to model predictions. This is of some importance, given the nature of predictions that are required of the Pavia groundwater model. As will be discussed in Section 5 of this document, these are probabilistic predictions of contaminant source status as a function of location. Consistency of particle path status that is ensured through history-matching ensures consistency of particle source status for any one parameter field. Probability maps can then be constructed by examining source statuses over many history-match-constrained parameter fields.

4. MODEL DETAILS

4.1 General

This section briefly describes construction and history-matching of the Pavia groundwater model.

The same modelling philosophy is adopted in construction of the Pavia groundwater model as is adopted in construction of models that are described in other GMDSI worked example reports. This philosophy is based on the premise that the task of groundwater modelling is to process groundwater data. The outcomes of this processing must be quantification and reduction of the uncertainties associated with predictions of management interest. We briefly remind the reader of two aspects of model design which can impel the modelling process to achieve these decision-support imperatives.

4.1.1 Structural Simplicity

A structurally simple model is a fast-running model; it is also numerically stable. This allows its use with PEST/PEST++. At the same time, it is less likely to contain hardwired hydrogeological details whose existence and particulars are uncertain. Ideally, site details that are uncertain should be represented stochastically; structure is not stochastic.

Naturally, there are limits on how simple the structure of a groundwater model can be. If a model's structure is too simple, its parameters may be required to adopt roles which compensate for its structural inadequacies. This can bias their estimated values; this, in turn, may bias the values of decision-critical model predictions. Ideally, the propensity for structurally-induced predictive bias can be included in quantified predictive uncertainty intervals. If the propensity for bias is less than uncertainty reductions accrued through simplicity-enabling history-matching, then the "uncertainty ledger" is in the black. See Doherty and Moore (2021) for further discussion.

The Pavia model employs a single layer. No attempt is made to simulate vertical variation of contaminant concentration in the subsurface. Nor is the discontinuous, perched, FFS aquifer represented. Simulation of perched conditions is fraught with numerical challenges; it slows simulation speed dramatically, and may precipitate numerical malperformance. Few details of the perched aquifer system, including the nature of discontinuities that establish its presence at some places but not at others, are known. We recognize that if hydraulic gradients in the perched system differ from those in the deeper system, its presence may introduce uncertainties that a single-layer model cannot quantify. We seek comfort in the fact that uncertainties associated with predictions of management interest are considerable (see the next section), and that perched conditions probably contribute little uncertainty in addition to that which we are able to quantify with a model that is structurally relatively simple.

The Pavia model simulates groundwater flow under steady state conditions. Hence seasonality of recharge is neglected. As is discussed below, temporal variations in head that the model does not attempt to replicate are represented as "noise" in steady-state head observations. Hence the steady-state assumption does not induce bias in model predictions; it simply inflates their uncertainties. This inflation is probably small compared with uncertainties incurred by information deficiency.

In 2017 a system of extraction wells was installed near the Navigliaccio Canal. This altered local groundwater gradients significantly. This is not simulated by the model that is described herein. We note, however, that the modelling and history-matching methodologies that we employ can accommodate temporal changes in groundwater gradients.

4.1.2 Parametric Complexity

Before the appearance of software such as PEST and PEST++, modellers were advised to adopt parameter parsimony as their guiding principle. Regularisation required to achieve parameter uniqueness was undertaken manually, and often in an ad-hoc fashion, using zones of piecewise constancy. As is documented by Doherty (2015), this type of regularisation is sub-optimal. It cannot be guaranteed to yield a parameter field that is of minimized error variance. Nor can an inversion process that is based on a simplistic parameter field be guaranteed to extract as much information from a history-matching dataset as that dataset contains.

Theoretically, there is no limit to the number of parameters with which a groundwater model can be endowed. As a model undergoes calibration, modern regularisation methods allow parameter uniqueness to be attained in ways that minimize the potential for parameter and predictive error. At the same time, the inversion process readily accommodates surprises as flexible parameterisation admits expression in estimated parameter fields of unexpected nuances of geology that a measurement dataset may reveal. Bredehoeft (2005) has drawn attention to the need for modellers to be attentive to surprises; he asserts that lack of such attentiveness has characterised the construction and deployment of many decision-support models.

As well as being carriers of information, parameters also perform an important role in expressing the repercussions of lack of information. When history-matching is undertaken probabilistically, the lack of estimability of individual or grouped parameters is expressed through their penchant for post-history-matching variability. This is made explicit when history-matching is undertaken using ensemble methods such as those supported by PESTPP-IES; their lack of estimability can also be quantified using linear analysis. If a prediction is sensitive to uncertain parameters, it inherits their uncertainties.

From a Bayesian point of view, the “golden rule” of model parameterisation can be summarized using the expression “if you do not know its value, then let it wiggle”. This applies to parameters that represent the spatial distribution of hydraulic properties. It also applies to parameters which represent quantities such as head and conductance that characterise model boundary conditions. If this precept is followed, it is incumbent on a modeller to attribute realistic prior probability distributions to these parameters.

4.2 Grid and Boundary Conditions

MODFLOW 6 is used to simulate movement of water within and around Pavia. MODPATH 7 is used for particle tracking.

Figure 4.1 depicts the model domain. The model employs a structured grid with uniform square cells with dimensions of 12.5 m × 12.5 m. Cell surface elevations are derived from a digital terrain model of the area. Cell bottom elevations are derived from a local geological model (Provincia di Pavia, 2021). (Note that errors in the assignment of bottom elevations to the FFB aquifer are unlikely to have a negative impact on model predictions, as all model predictions of interest rely on transmissivity rather than individually on hydraulic conductivity and aquifer depth. Once aquifer bottom elevations have been assigned, it is transmissivity that is effectively estimated through history-matching.)

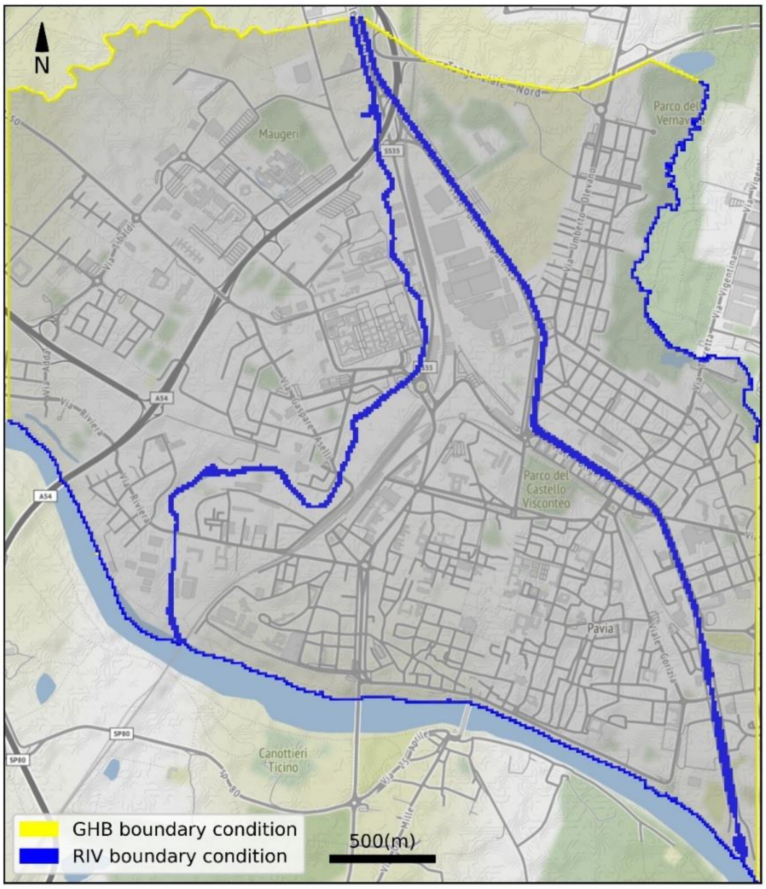

Figure 4.1. Domain and boundary conditions of the Pavia model.

The southern boundary of the model follows the Ticino River. This is simulated using the MODFLOW river (i.e. RIV) boundary condition. A RIV boundary condition also represents the Roggia Vernavola Canal along the northeastern model boundary, and the Naviglio di Pavia and Navigliaccio Canals which lie within the model domain. History-match-adjustable heads and conductances are assigned to all of these boundaries; see below.

The remaining portions of the boundary (that is, the northern boundary, and the straight boundary segments along the eastern and western margins of the model domain) are denoted as general head boundaries (i.e. GHBs). As for the RIV boundaries, their heads and conductances are decreed to be adjustable; they are therefore inferable through calibration, and constrained by stochastic history-matching. Initial values of heads along GHB boundaries were set equal to land surface elevations. These heads thus represent conditions at unspecified locations outside of the model domain. Meanwhile, boundary conductances represent the hydraulic connection of the model domain to these distant points. Water loses head as it flows through this connection.

It should be noted that the history-matching process that is described below assigned values to GHB head and conductance parameters that yield realistic values for model-calculated heads just inside these boundaries. Reasonable values for depth to groundwater were obtained (mostly between 5 and 15 metres). Meanwhile flow along the eastern and western boundaries was calculated to be roughly parallel to these boundaries. If this were not the case, the history-matching dataset could have been supplemented with "observations" of reasonable groundwater behaviour at these boundaries in order to establish these conditions. However this was not found to be necessary.

The following should also be noted:

- Lateral model boundaries are far enough away from contaminant sources and measurement points (especially the model's eastern and western boundaries) for them to have little influence on model calculations of interest.
- Adjustment, rather than direct assignment, of boundary conditions recognises their uncertainties. These uncertainties can thereby be transferred to model predictions. Uncertainties of the latter are not therefore understated.

As a further precaution against aberrant groundwater behaviour in a modelling environment characterised by a high level of parameter stochasticity, all cells within the model domain are equipped with a drain (i.e. DRN) boundary condition. DRN elevations are set at the land surface while DRN conductances are set to very high values. This allows water to find its own point of escape from the groundwater system in low-lying parts of the model domain should it need to do so. In practice, this occurs at only a few locations that are close to rivers and canals.

Recharge is applied to every cell within the model domain. Like hydraulic conductivity, it is spatially parameterised and adjustable.

4.3 History-Matching

4.3.1 General

Prior to being used for probabilistic contaminant source assessment, the Pavia model was subjected to two kinds of history-matching. First it was calibrated. Calibration seeks a unique solution to the inverse problem posed by fitting model outputs to field measurements. This problem is inherently nonunique. Uniqueness of a calibrated parameter field is attained through numerical regularisation which, in general, minimizes parameter departures from a set of preferred values or conditions such as smoothness or homogeneity. It can be shown that minimization of an appropriately defined objective function that studiously balances model-to-measurement misfit (encapsulated in a "measurement objective function") against departures from a preferred parameter condition (encapsulated in a "regularisation objective function") attains parameter uniqueness.

Programs such as PEST_HP implement algorithms which are able to balance the measurement and regularisation components of an objective function in a way that ensures that model-to-measurement fit is good, but not excessive. At the same time, they support innovative definition of the regularisation objective function. The latter can take advantage of covariance matrices that define spatial correlation between parameters; if desired, spatial correlation can be spatially variable. See Doherty (2015) and GMDSI training material for further details. Inclusion of these matrices in definition of the regularisation objective function ensures that history-match-emergent patterns of heterogeneity are "spread out" rather than "spotty".

The second type of history-matching to which the Pavia groundwater model was subjected is stochastic. The PESTPP-IES ensemble smoother was employed to calculate a suite of parameter fields, all of which minimize the measurement component of the objective function. As for PEST_HP, mechanisms are put in place to prevent over-fitting of model outputs to measurements comprising the history-matching dataset. Meanwhile, hydrogeological integrity of the history-match-constrained ensemble of parameter fields is ensured by adjusting an initial set of parameter realisations that sample an appropriately-defined prior parameter probability distribution. This prior parameter probability distribution can employ the same set of covariance matrices as those that are used for parameter regularisation; alternatively, it can employ matrices that are derived from them.

Theoretically, realisations which comprise the initial parameter ensemble that is adjusted by PESTPP-IES should be sampled from the prior parameter probability distribution. In stochastic history-matching of the Pavia model, computing time was saved, and a superior fit between model outputs and the history-matching dataset was attained, by following these steps:

1. The Pavia model was first calibrated using PEST_HP. This allowed a good fit between model outputs and field measurements to be attained with a parameter field that is relatively smooth, and that therefore appears to be relatively free of signs of parameter compensatory behaviour. This constitutes validation of the novel history-matching workflow that is described in the previous section.
2. Based on this parameter field, a posterior parameter covariance matrix was evaluated using sensitivities calculated by PEST_HP. This allows formulation of a linear approximation to the posterior parameter probability distribution.
3. Three hundred parameter realisations were sampled from this distribution.
4. These realisations were adjusted by PESTPP-IES to fit the history-matching dataset. Adjusted realisations comprise samples of the posterior parameter probability distribution.

4.3.2 Parameters

4.3.2.1 Pilot Points

Parameterisation of the Pavia model makes extensive use of pilot points.

Figure 4.2 shows pilot points which are used for parameterization of hydraulic conductivity, recharge and porosity. In all, there are 628 of these. Pilot points are emplaced with high spatial density where observation wells are spatially dense. Their emplacement is spatially more frugal in outer portions of the model domain where observation wells are sparse or absent.

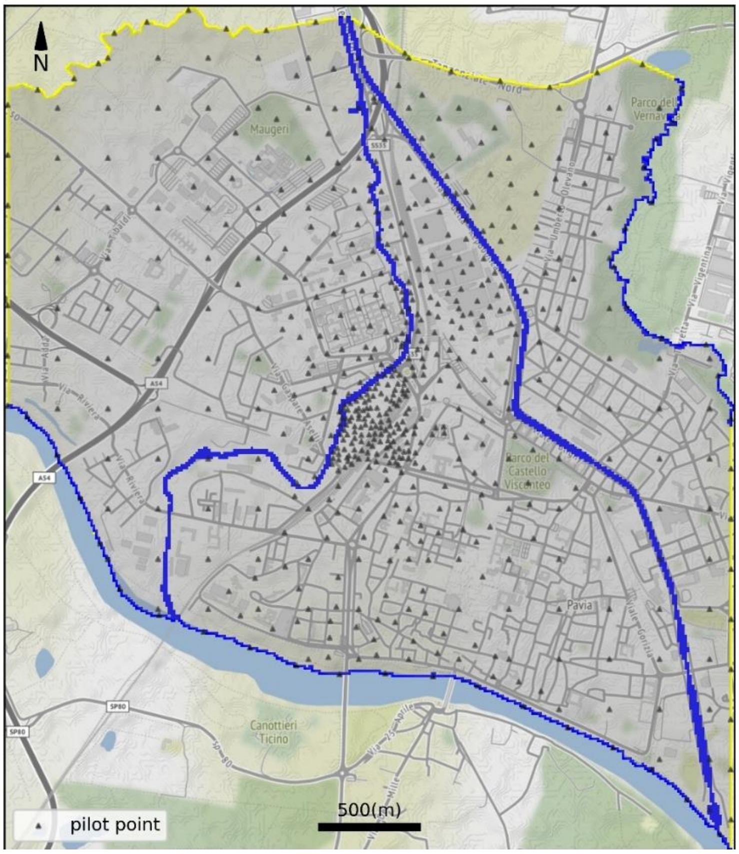

Figure 4.2. Pilot points used for parameterisation of hydraulic conductivity, recharge and porosity.

Figure 4.3 shows pilot points to which boundary condition parameters are assigned. These are emplaced along surface waterways (rivers and canals) that are represented using RIV boundary conditions, and along those portions of model lateral boundaries to which GHBs are ascribed. Density of pilot point emplacement is relatively uniform along these boundaries, except for RIV pilot points in areas of high observation well density; a higher spatial density of pilot point emplacement prevails in the latter areas.

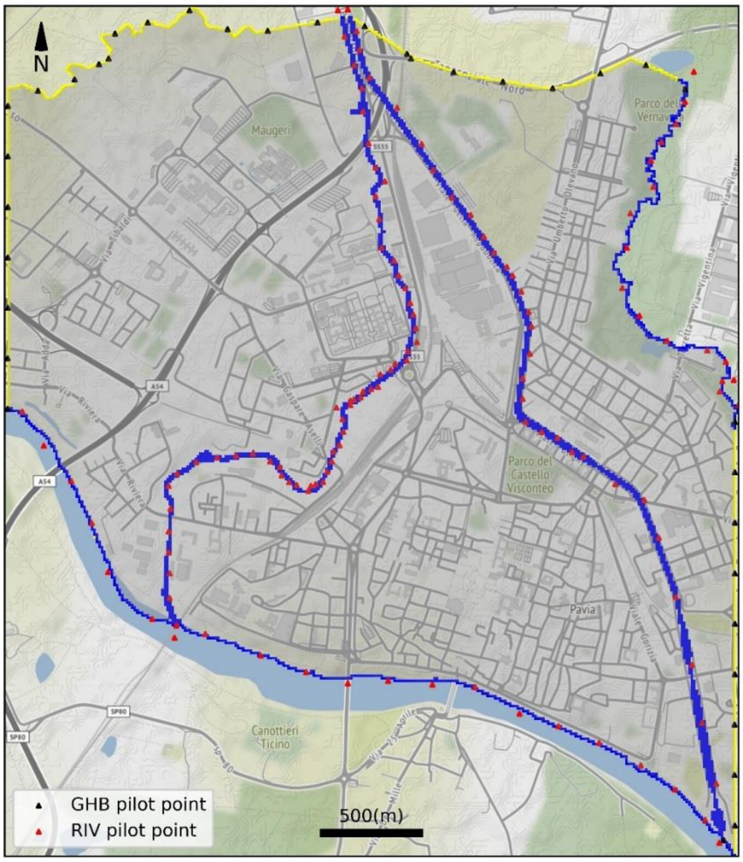

Figure 4.3. Pilot points which are used for boundary condition parameters.

4.3.2.2 Hydraulic Conductivity

Prior to calibration, an initial value of 17 m/d was assigned to all hydraulic conductivities. This is the geometric average of hydraulic conductivities calculated from analyses of local pumping tests. A prior covariance matrix for the log of hydraulic conductivity was calculated using the MKPPSTAT and PPCOV_SVA utilities supplied with the PEST Groundwater Utility Suite. These allow spatial correlation to vary with pilot point density. A log (to base 10) standard deviation of 0.5 was ascribed to all hydraulic conductivity pilot point parameters.

4.3.2.3 Recharge

Initial values for recharge pilot point parameters are uniformly 200 mm/yr. A covariance matrix based on a spatially variable correlation length was constructed in the same manner as for hydraulic conductivity parameters. A prior standard deviation of 75 mm/yr was ascribed to all recharge parameters.

4.3.2.4 Porosity

Porosity has no effect on particle trajectories. However, it affects their travel times. The lower is the porosity, the faster does a particle move.

In the Pavia model, particles are allowed to travel for up to 50 years through a steady state flow field. This spans the time over which contaminants are thought to have leaked into the local groundwater system. Termination of an aged particle's trajectory before it reaches the southern boundary of the model domain can affect its detect/nondetect/inconsistency status; this affects the status of the model cell in which the particle is released. However this effect is minor because there are few observation wells near the model's southern boundary.

When calibrating the Pavia model, porosity was assigned a uniform value of 0.2. When undertaking uncertainty analysis, a value of 0.05 characterises its standard deviation.

4.3.2.4 RIV Boundary Conditions

Two parameters are associated with each RIV pilot point. The first of these is conductance. RIV conductance parameters were all awarded an initial value of 1 m^2/d, a log-standard deviation of 0.5, and a spatial correlation length that is slightly greater than the local inter-pilot-point distance.

The most downstream pilot point of each RIV boundary segment is ascribed an initial value of head that is appropriate for its location; this head is history-match-adjustable within a narrow range. Pilot points upstream from these are assigned Δh parameters; these denote the head increment from the nearest downstream pilot point. Values of Δh are endowed with a lower bound of zero; this ensures downhill flow of water. Initial values of Δh are location-dependent; where necessary, they account for the presence of dams and lochs. Standard deviations (applied to the log of Δh values) are uniformly 0.25.

4.3.2.5 GHB Boundary Conditions

Conductance parameterization of GHBs follows a similar strategy to that of RIVs. The initial conductance is uniformly 0.1 m^2/d, while the log-standard deviation is 0.5. A spatial correlation length that is slightly greater than the local inter-pilot-point distance is employed.

Initial heads assigned to GHBs are land surface elevations at respective pilot point locations. Thus the boundaries represent conditions at some distance from the model domain, while boundary conductances represent hydraulic connections to these distant points. A drop in hydraulic head is experienced as water flows through these connections. A spatial correlation length that is slightly greater than the local inter-pilot-point distance is employed for conductance parameters.

4.3.3 Observations

4.3.3.1 Heads

Between 2004 and 2016, a number of head measurements were made in observation wells that are depicted in Figure 2.2. Head measurements pertaining to each well were averaged to obtain a "steady state" head for that well. The standard deviation of these measurements quantifies "measurement noise". The inverse of this standard deviation is used to weight the respective steady state head observation during model calibration. The PESTPP-IES ensemble smoother uses this standard deviation to generate random realisations of measurement noise as it adjusts parameter fields to accommodate steady state head measurements.

4.3.3.2 Particle Inconsistency

The use of particle tracks in Pavia model history-matching is described in Section 3. "Observations" of zero inconsistency are associated with all particles that are used in calibration of the Pavia model. Weights used in history-matching ensure visibility of this component of the measurement objective function. This incentivises PEST_HP and PESTPP-IES to fit these observations by calculating parameters that ensure particle track consistency. As is discussed in the previous section, this provides a mechanism for assimilation of information that is resident in borehole measurements of contaminant concentration.

4.3.3.3 Surface Water Elevations

Canal and river levels have been measured at 39 locations. As is explained above, the modelled elevations of surface water bodies are subject to calibration adjustment under the constraint that water flows downhill. Inclusion of direct measurements of surface water level in the history-matching dataset further constrains history-match-estimated surface water elevations.

4.3.3.4 Flow from Drains

Deployment of the MODFLOW DRN boundary condition is discussed in Section 4.2. Its use is complemented by a set of “observations” that water does not escape from the groundwater system through these drains; they thus comprise a “boundary condition of last resort”. The model domain is subdivided into a grid of 50 rectangles of approximately equal area in which flow from DRN boundary conditions is computed. “Observed” values of all of these flows are zero.

This strategy maintains sensibility of model-computed piezometric heads as parameters are adjusted, at the same time as it allows water to escape from the groundwater system where this cannot be avoided because of low topographic elevation. Precautions such as this are sometimes necessary when the many uncertainties that are associated with construction of a groundwater model are recognised in a parameterisation strategy that allows expression of these uncertainties.

4.4 History-Matching Outcomes

4.4.1 General

In the interests of brevity, only a few outcomes of the history-matching process are presented herein. The outcomes of probabilistic capture zone analysis, which is the subject of the next section, are far more exciting.

4.4.2 Calibration

Figure 4.4a depicts the hydraulic conductivity field achieved through model calibration, while Figure 4.4b depicts the calibrated recharge field. As expected, these are relatively smooth as they comprise minimum error variance solutions to an ill-posed inverse problem.

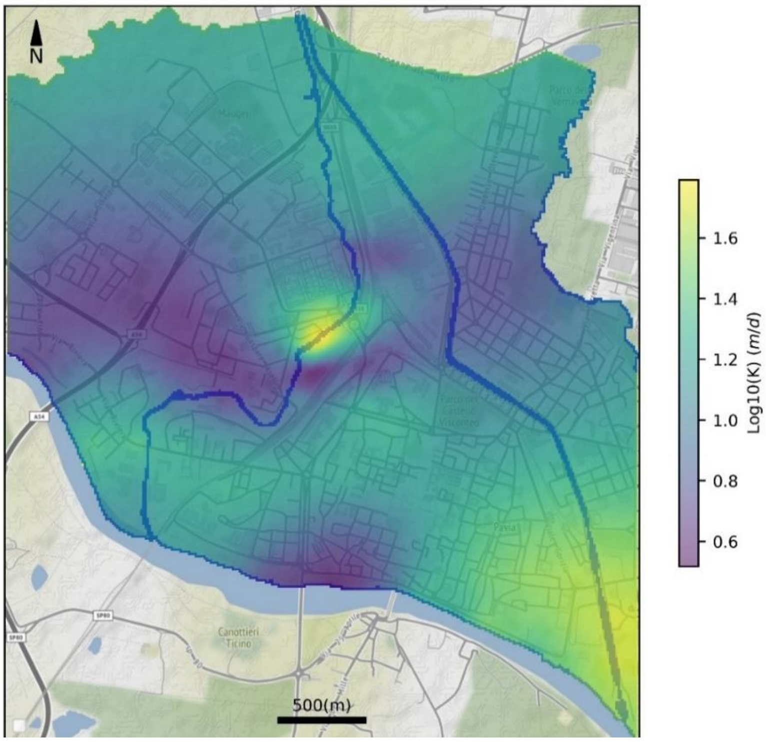

Figure 4.4a. Calibrated hydraulic conductivity.

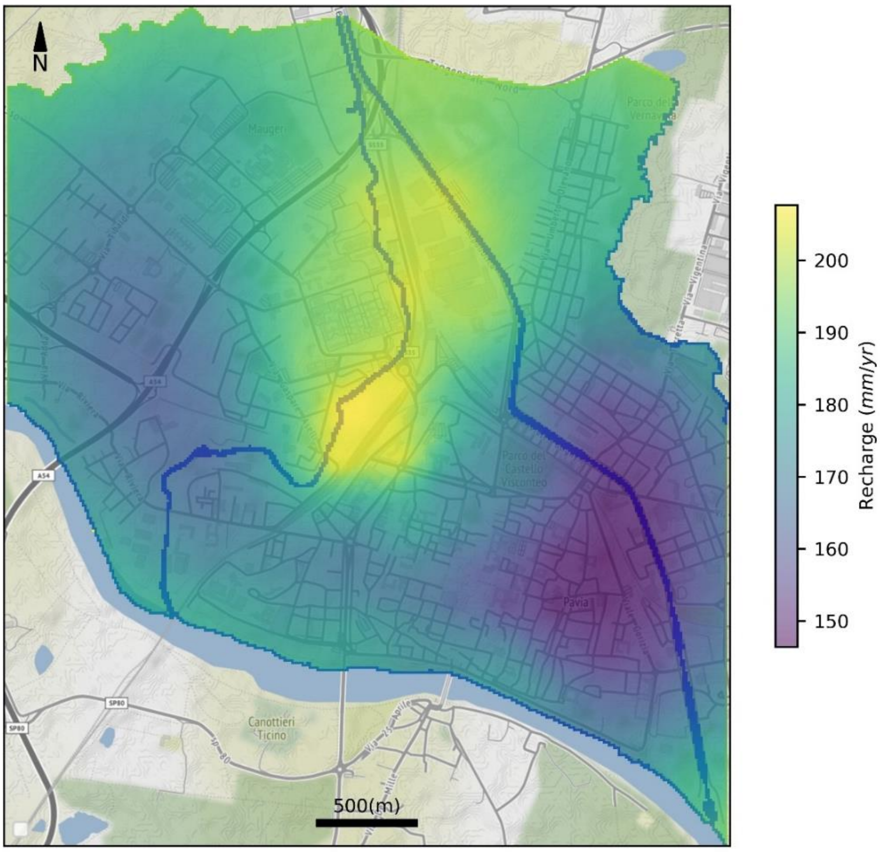

Figure 4.4b. Calibrated recharge.

Some heterogeneity of hydraulic conductivity is visible in the vicinity of measurement wells. It is unlikely that the hydraulic conductivity of the FFB aquifer is either homogeneous or smoothly varying in other parts of the model domain. However, heterogeneity can only be inferred where measurements of system behaviour that are reflective of its presence are available.

Heads throughout the model domain as calculated by the calibrated model are shown in Figure 4.5. This figure also depicts particles that are endowed with a non-zero detect status. Naturally, these particles pass close to wells in which PCE was detected.

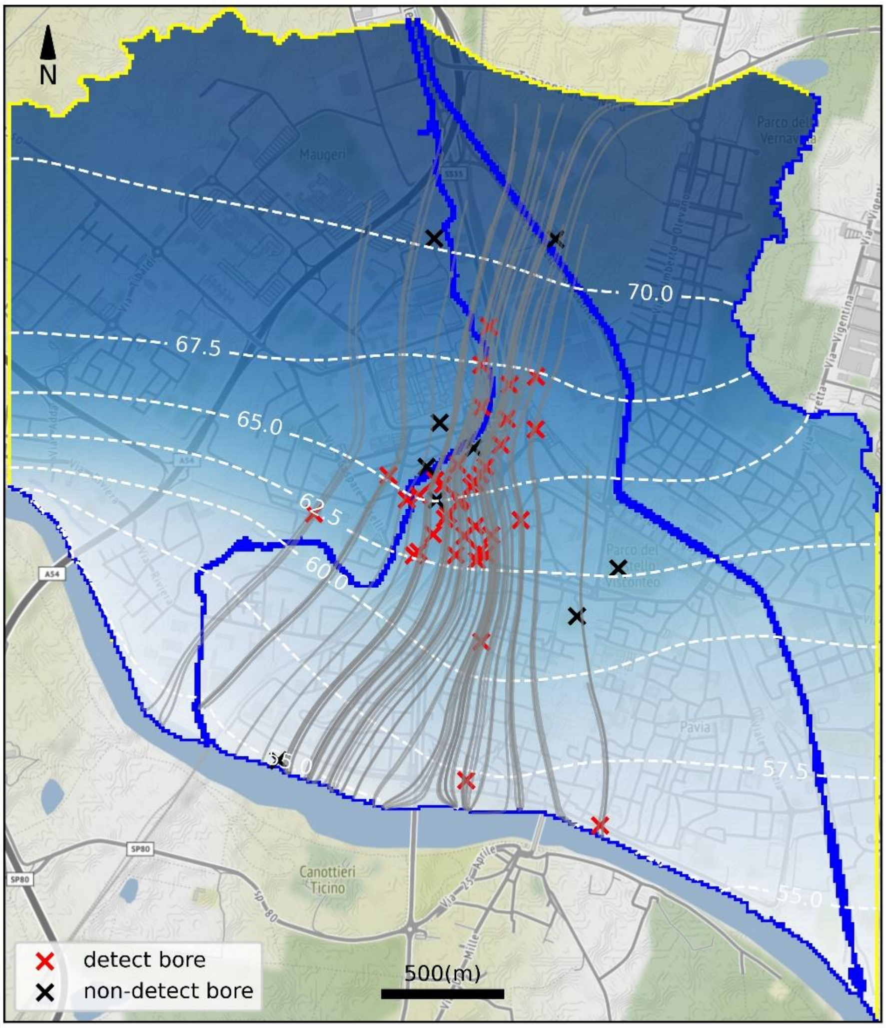

Figure 4.5. Piezometric heads calculated using the calibrated model. Particle tracks with a non-zero detect status are also shown.

4.4.3 Ensembles

A total of 300 parameter fields comprises the ensemble that was adjusted by PESTPP-IES. All of these attain a fit with the observation dataset that is commensurate with that attained by PEST_HP. Nine history-match-constrained hydraulic conductivity fields are presented in Figure 4.6a while nine history-match-constrained recharge fields are presented in Figure 4.6b. Nine realisations of porosity are presented in Figure 4.6c; as is discussed above, porosity realisations undergo very little adjustment as the constraints imposed on them by field data are small.

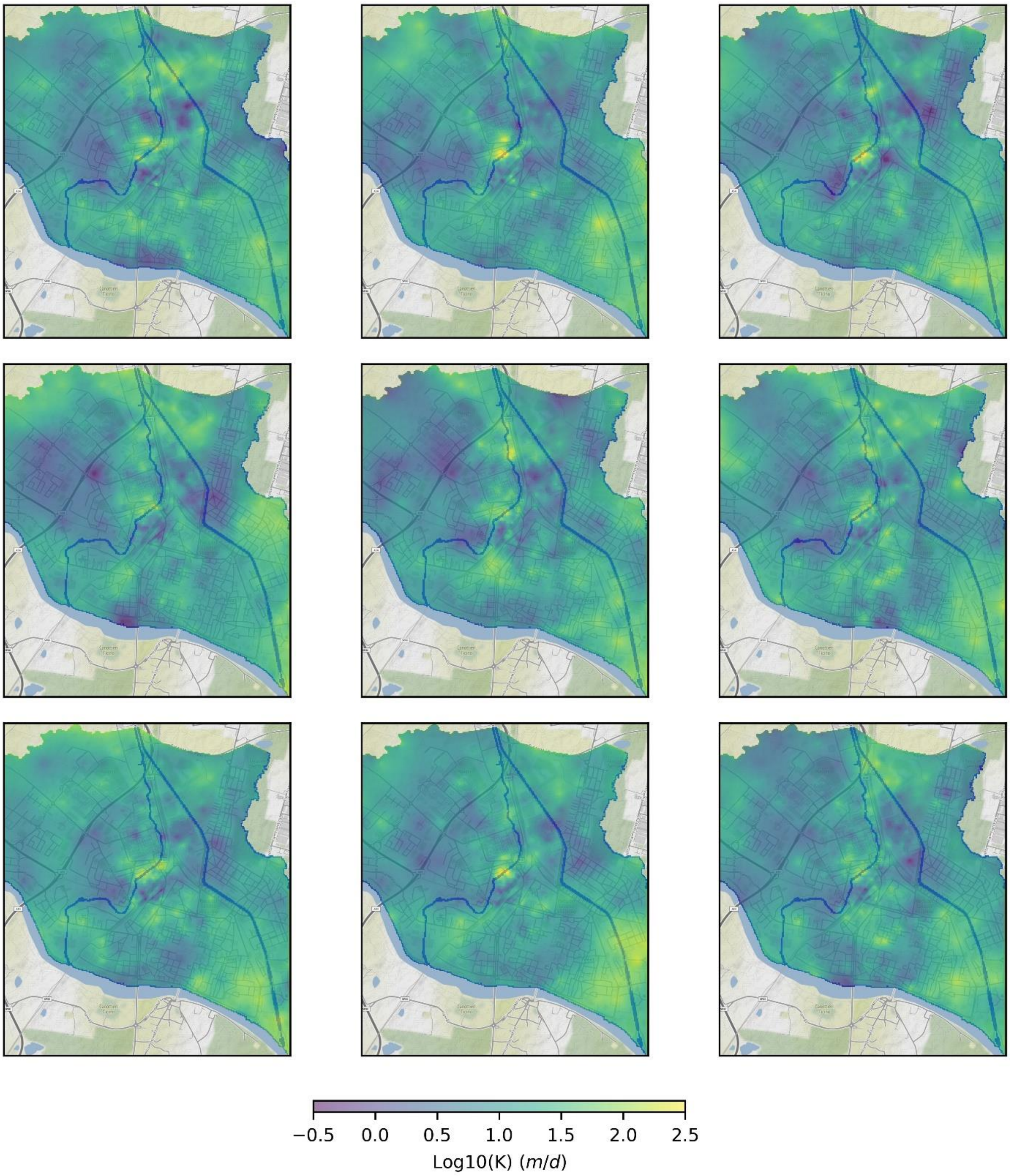

Figure 4.6a. Nine realisations of history-match-constrained hydraulic conductivity.

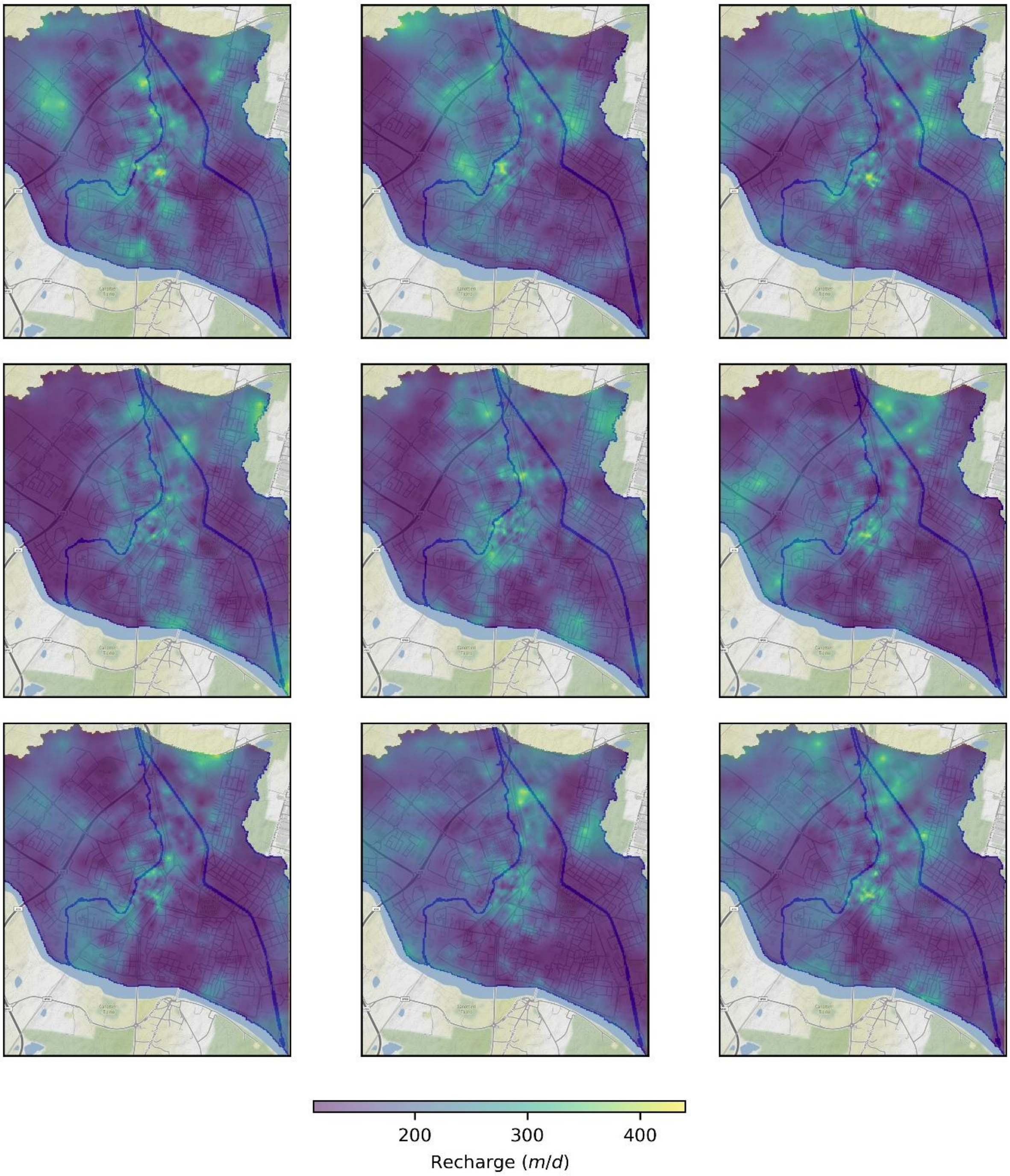

Figure 4.6b. Nine realisations of history-match-constrained recharge.

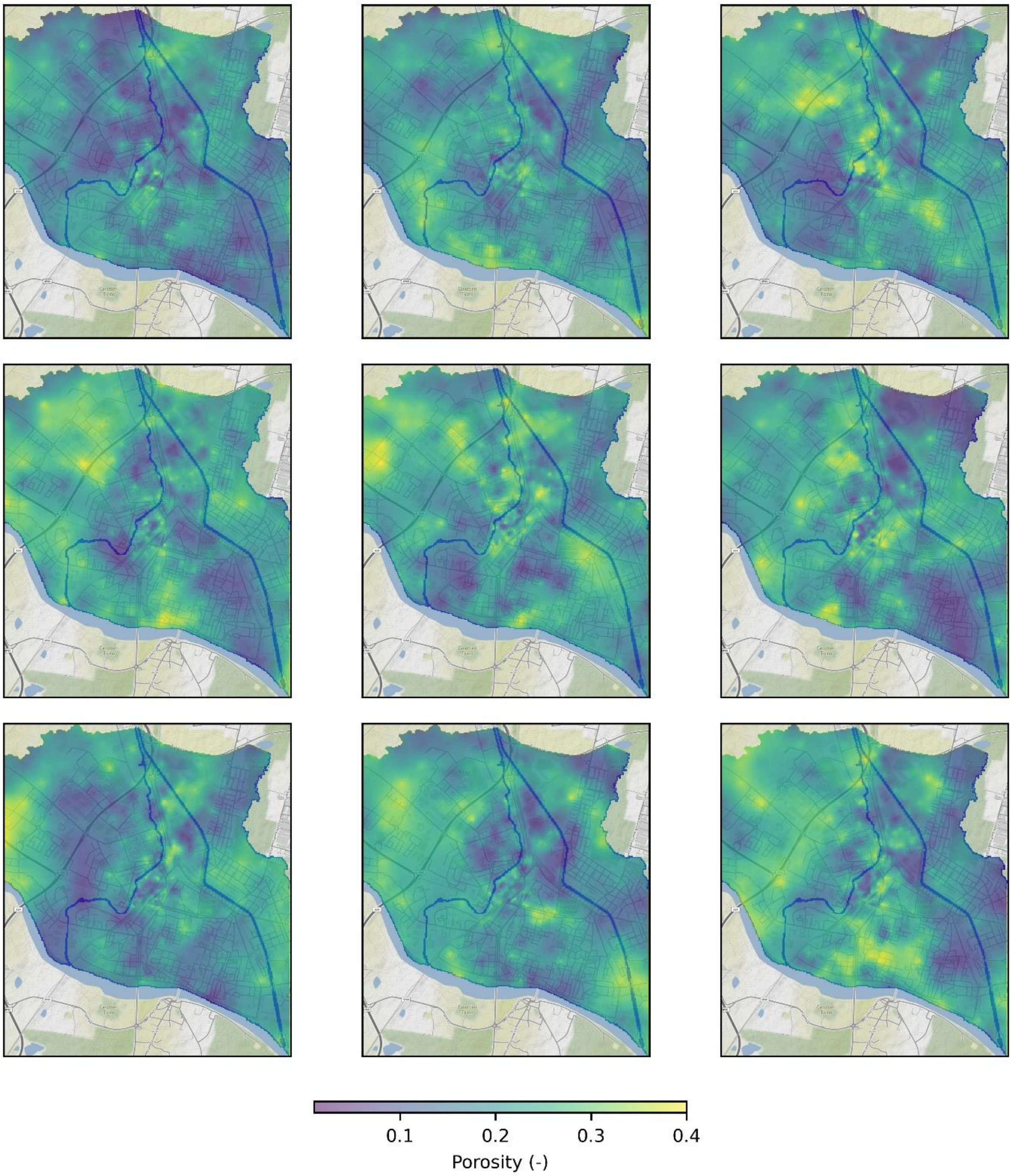

Figure 4.6c. Nine realisations of history-match-constrained porosity.

Figure 4.7a presents the standard deviation of the log (to base 10) of hydraulic conductivity in all model cells, while Figure 4.7b depicts the standard deviation of recharge. The standard deviation is calculated over all members of the history-matched ensemble.

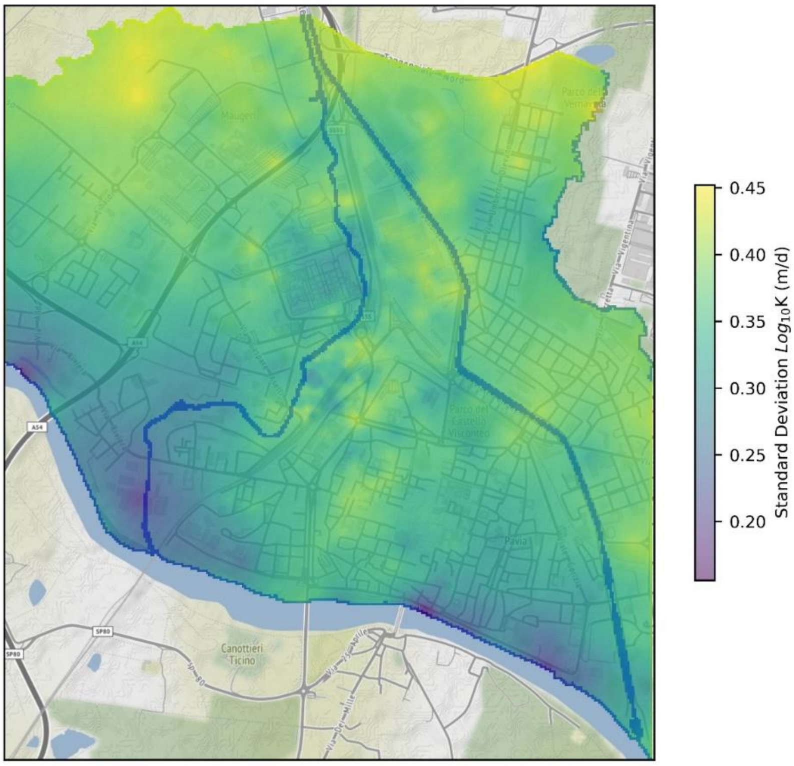

Figure 4.7a. Posterior standard deviation of hydraulic conductivity.

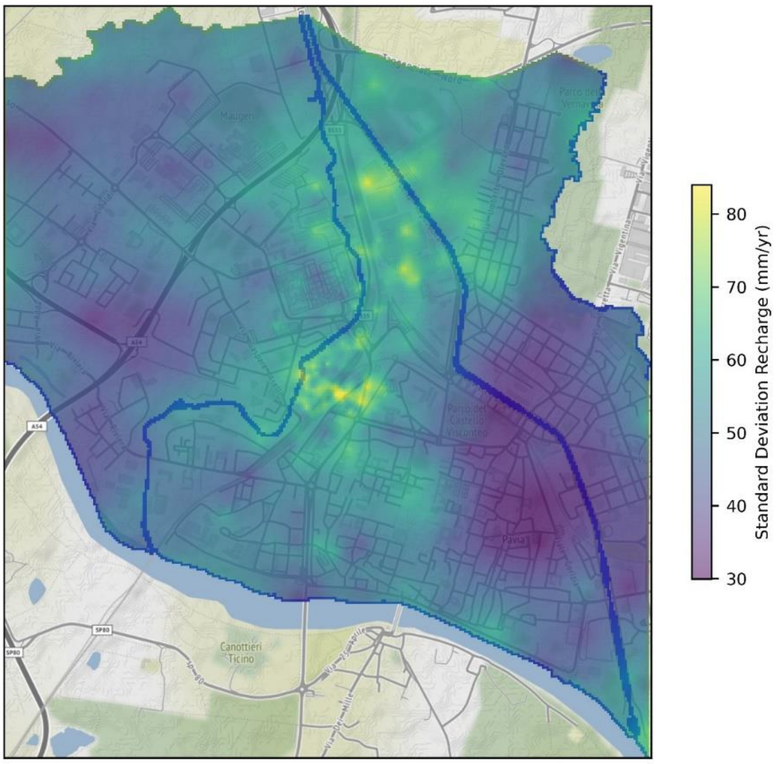

Figure 4.7b. Posterior standard deviation of recharge.

5. MODEL PREDICTIONS

5.1 Contaminant Source Statistics

5.1.1 Detect Status

Section 3 of this document describes how post-processing of particle tracks can confer on each particle that is released within the domain of a model three separate statuses, namely a detect status, a nondetect status and an inconsistency status. History-matching ensures that if a particle has a nonzero detect status, then its nondetect status cannot also be significantly nonzero (and vice versa). A particle can therefore possess either a positive detect status, or a positive nondetect status. Alternatively, both of these statuses can be zero; this occurs if the particle does not pass near an observation well.

Section 3 also explains how the detect status of a particle is transferred to the cell in which the particle originates. For a given parameter field, each cell within the model domain is therefore assigned a detect status, a nondetect status, or neither of these statuses. History-matching ensures that the inconsistency status of all model cells is zero or minimal.

The PESTPP-IES ensemble smoother history-matched the Pavia groundwater model 300 times. In each of the parameter fields that emerged from this process, different particles may pass close to different observation wells; their statuses may therefore vary from parameter field to parameter field. It follows that the statuses of cells in which particles are released may vary from parameter field to parameter field. This variability can be characterized statistically. The resulting statistics are informative of contaminant source probability.

The outcomes of statistical analyses that are shown in this section are based on the “best” 150 parameter fields out of the 300 parameter fields that were adjusted by PESTPP-IES. “Best” is defined on the basis of the component of the objective function that measures particle inconsistency; the lower is this component of the objective function, the “better” is the corresponding parameter field deemed to be. (It should be noted, however, that repetition of these analyses using all 300 parameter fields yields results that are only marginally different from those that are depicted below.)

The average detect status of any model cell can be computed by summation of its detect status over all stochastic parameter realisations, and then dividing by the number of realisations. This is a measure of the likelihood of detection of a contaminant by the current observation network if a contaminant source exists in that cell. Presumably, the prior probability of a contaminant source existing in any cell can be obtained from land use and other records.

The authors of this report do not possess the knowledge required to construct a prior contaminant source probability map. So we choose an alternative way of depicting the average detect status of model cells. If the average detect status of an individual cell is subtracted from 1.0, the result expresses the probability that a contaminant released in that cell will be undetected by the current observation network. These probabilities are mapped in Figure 5.1. It is apparent from this map that the probability of a contaminant source going undetected approaches zero (coloured blue in this figure) in cells that are immediately upgradient of wells in which contaminant has actually been detected.

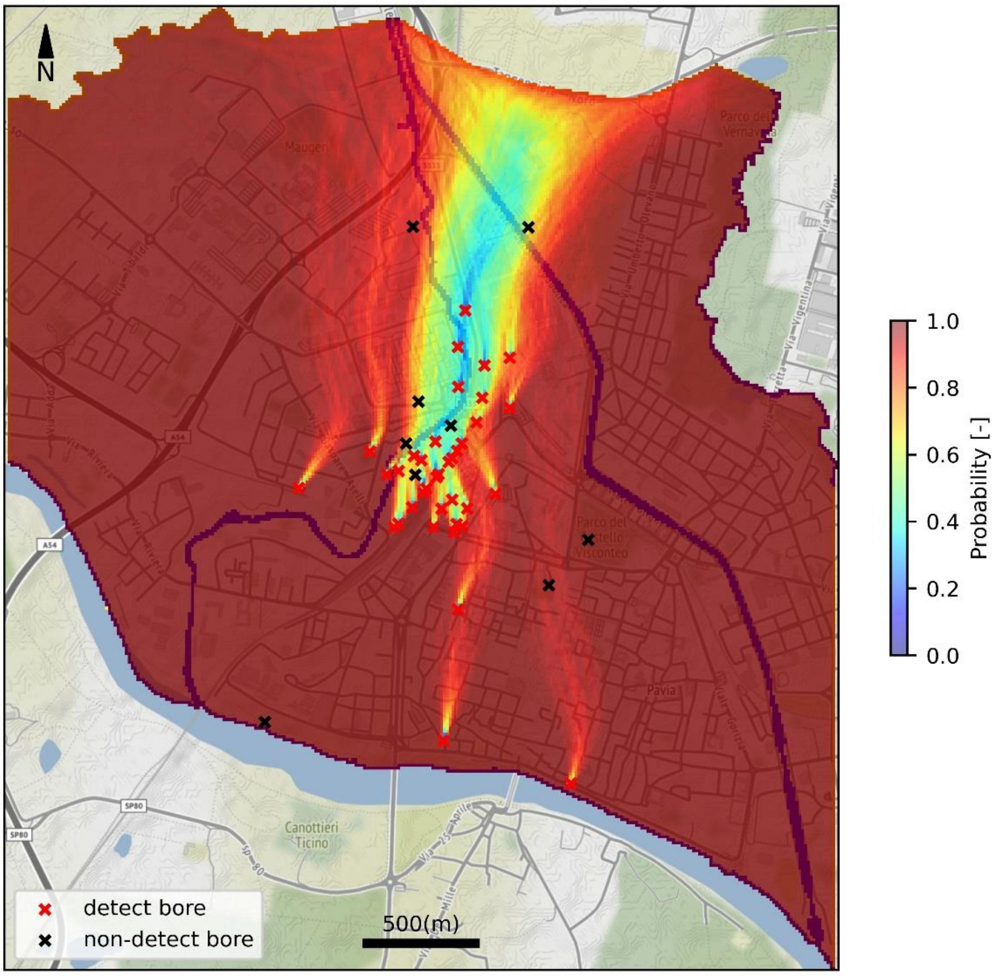

Figure 5.1. Probability that a contaminant source at a particular location is undetected by the present observation network.

5.1.2 Nondetect Status

In similar fashion, the nondetect status of any cell can be averaged over all parameter realisations. This yields the probability that a contaminant source does not exist in that cell. This probability is mapped in Figure 5.2. In order to facilitate comparison with Figure 5.1, high levels of nondetect status are coloured blue in this figure. This is a stronger statistic than that described in the previous subsection. Hence the bands of significantly high probability are narrower than the bands of low probability that are depicted in Figure 5.1. (Both are coloured blue.) It is apparent that certainty of nonexistence of a contaminant source prevails only in cells that are immediately upstream of nondetect wells.

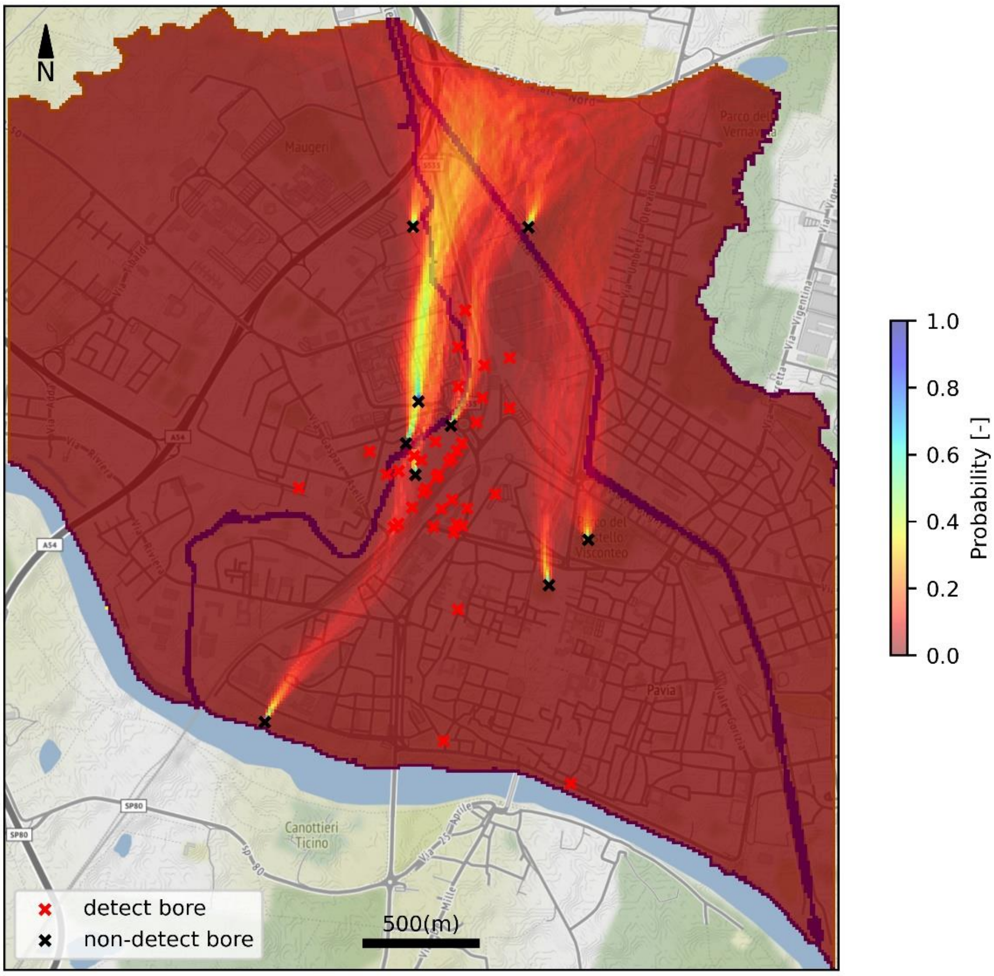

Figure 5.2. Probability that a contaminant source does not exist at a particular location.

5.2 Data Acquisition

5.2.1 Background

The question often arises, "what data should be gathered next?". Modelling and concepts that are discussed above can answer this question.

The worth of data rises in proportion to its ability to reduce the uncertainties of predictions that matter. In the present case, predictions that matter pertain to contaminant source locations. Hence the worth of data increases in proportion to their ability to reduce the uncertainties of these inferred locations.

Suppose that we wish to explore the possibility that a contaminant source is located somewhere within the polygon that it depicted in Figure 5.3. Suppose further that we must select between two proposed observation wells. Intuitively, the closer is an observation well to a polygon of interest, the greater is its information content with respect to that polygon. However, the observation well may inform only a part of the polygon because of its proximity to that part. Information gleaned from a well that is further away from the polygon may be more thinly spread over the polygon; however this information may span more of its area. Much will depend, of course, on the path that groundwater takes prior to reaching the proposed observation well. This is uncertain. It is affected by uncertainties in local hydraulic conductivity and by uncertainties in nearby boundary conditions. These uncertainties have been captured and reduced by PESTPP-IES; they are represented in parameter realisations that it has calculated and constrained.

Two proposed observation wells are depicted in Figure 5.3. We will refer to these as the "northern well" (N) and the "southern well" (S).

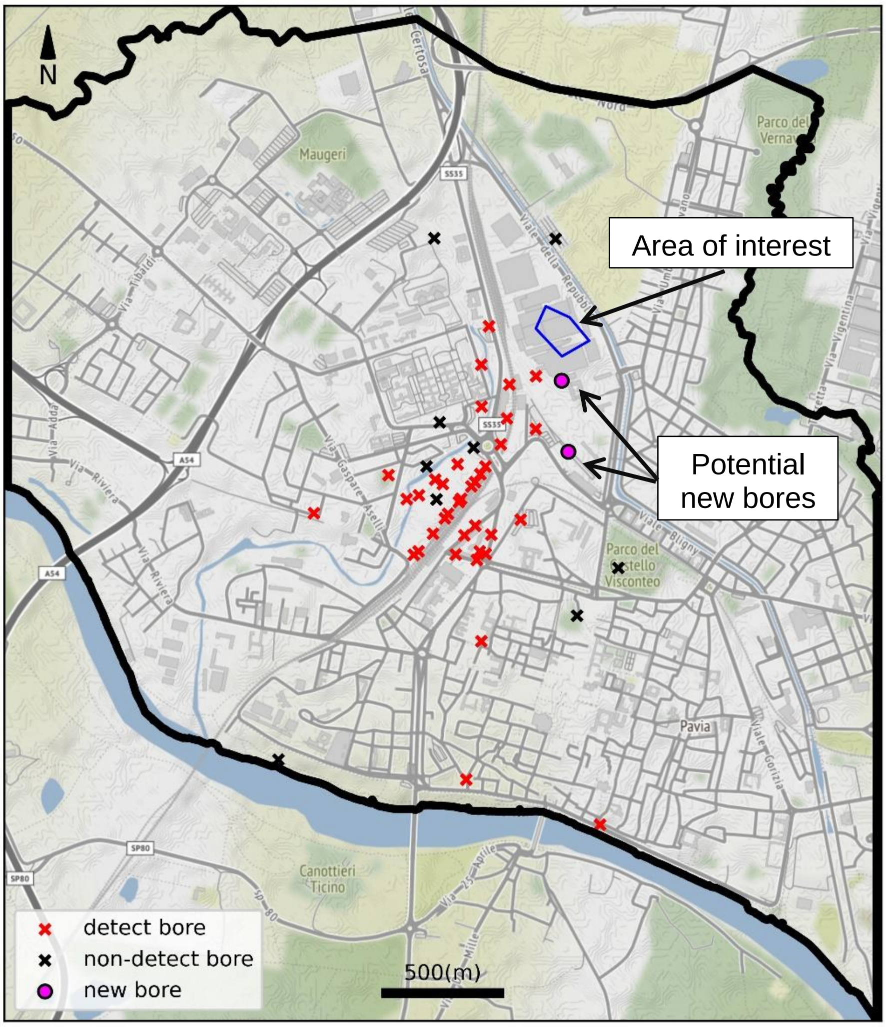

Figure 5.3. Area of interest and new observation wells.

5.2.2 Procedure

Before outlining a procedure through which the comparative worth of the two proposed observation wells can be evaluated, we provide some definitions. These make the following discussion easier to understand. We define the spatially-varying probabilities that are mapped in Figures 5.1 and 5.2 respectively as "probability of source non-detection" or "P_{SND}", and "probability of source nonexistence" or "P_{SNE}".

The procedure is now described. Note that stochastic particle trajectories that have already been calculated for the Pavia groundwater model can be used for this analysis. The model does not need to be re-configured, nor undergo any further history-matching.

1. Re-calculate detect and nondetect probabilities for all particles for all PESTPP-IES-calculated parameter fields under two opposing assumptions for each proposed observation well. This results in the calculation of four new sets of statistics. The opposing assumptions for each observation well are that:
    a. the proposed well detects contaminated groundwater;
    b. the proposed well does not detect contaminated groundwater.

2. Transfer particle statistics to their source cells and average them over all realisations. Thereby obtain P_{SND} and P_{SNE} for each cell.
3. Of particular interest are P_{SND} and P_{SNE} for cells which lie within the polygon of interest. These should be averaged over the polygon. Eight statistics can thereby be assigned to this polygon. These are:
    a. P_{SND}^{ND}; this is P_{SND} averaged over the polygon of interest under the assumption that the proposed northern well detects a contaminant (ND).
    b. P_{SND}^{NN}; this is P_{SND} averaged over the polygon of interest under the assumption that the proposed northern well does not detect a contaminant (NN).
    c. P_{SND}^{SD}; this is P_{SND} averaged over the polygon of interest under the assumption that the proposed southern well detects a contaminant (SD).
    d. P_{SND}^{SN}; this is P_{SND} averaged over the polygon of interest under the assumption that the proposed southern well does not detect a contaminant (SD).
    e. The same set of four statistics for P_{SNE}.

The absolute value of the difference $\left|P_{SND}^{ND} - P_{SND}^{NN}\right|$ is a measure of the information content of the proposed northern well. It specifies the difference in the probability that a contaminant source will go undetected, integrated over the polygon of interest, that would prevail if, on the one hand, a contaminant is detected in the northern well and if, on the other hand, a contaminant is not detected in the northern well. By comparing this with the same statistic for the southern well, namely $\left|P_{SND}^{SD} - P_{SND}^{SN}\right|$, the worth of these two wells can be compared. $\left|P_{SND}^{ND} - P_{SND}^{NN}\right|$ for the northern well is calculated to be 0.058; its maximum possible value is 1.0. $\left|P_{SND}^{SD} - P_{SND}^{SN}\right|$ for the southern well is calculated to be 0.020. By this measure, the northern well is clearly superior.

Figure 5.3a shows P_{SND} calculated over the model domain under the assumption that the proposed northern well detects contaminants. If the proposed northern well does not detect contaminants, the map is very similar to Figure 5.1. (This is an outcome of the fact that the proposed well is situated some distance to the east of the existing monitoring network; its existence has little effect on statistics that are calculated using this monitoring network.) Figure 5.3b shows P_{SND} calculated over the model domain under the assumption that the proposed southern well detects contaminants. If the proposed well does not detect contaminants, the resulting map is also similar to that shown in Figure 5.1.

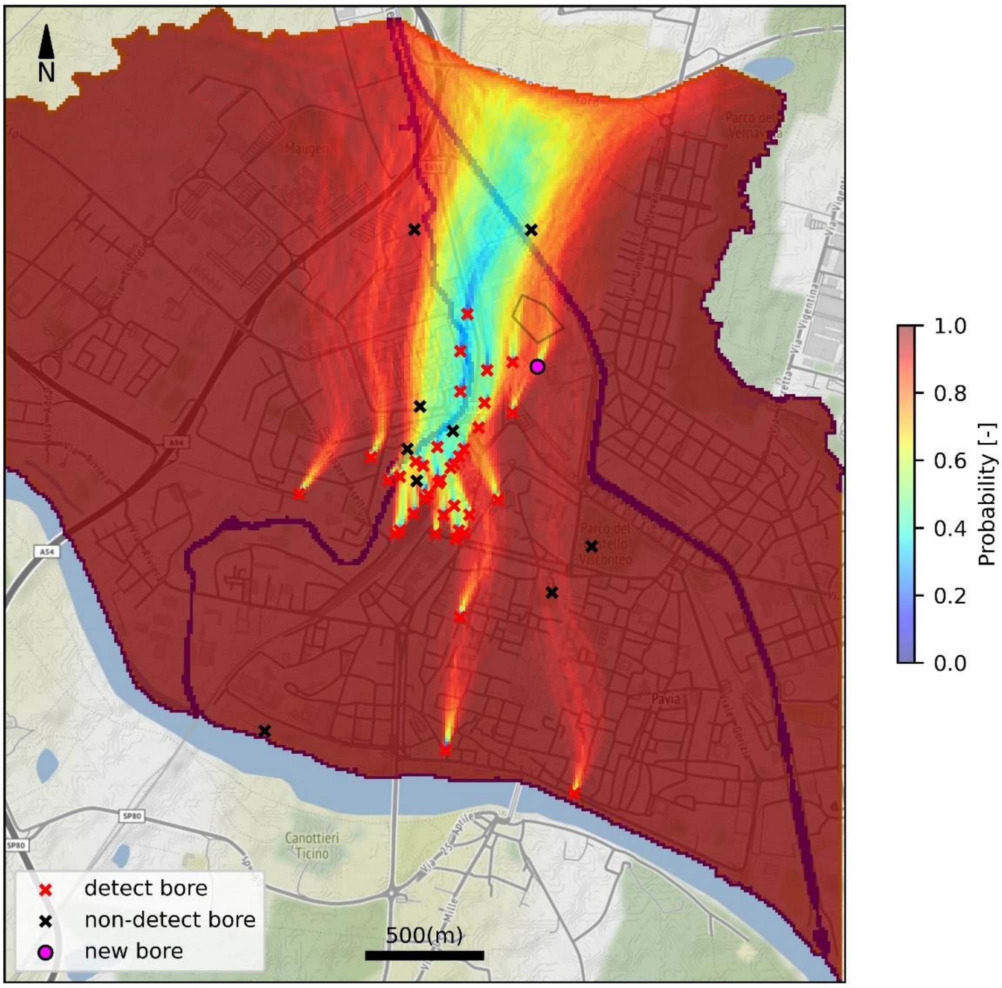

Figure 5.3a. Distribution of P_{SND} under the assumption that the proposed northern well detects contaminants.

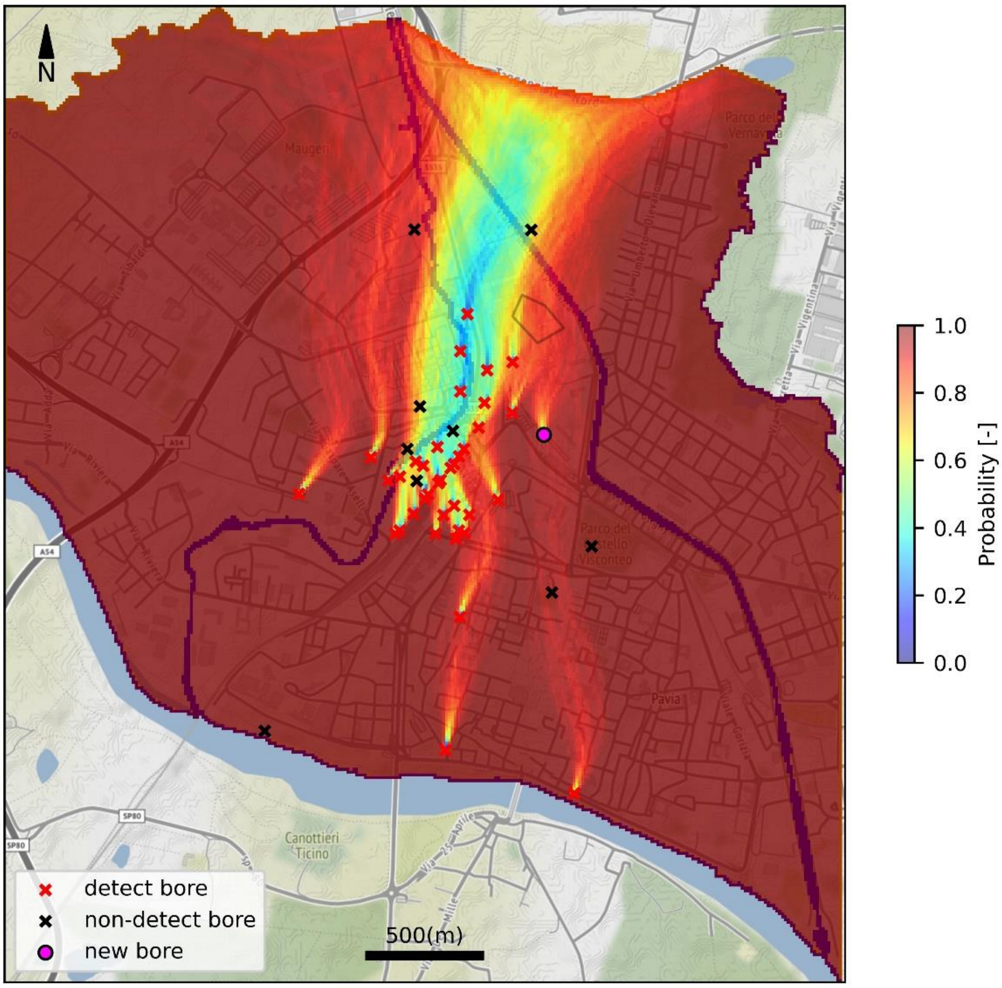

Figure 5.3b. Distribution of P_{SND} under the assumption that the proposed southern well detects contaminants.

The same procedure can be repeated using the P_{SNE} statistic. If this is done, it can be established that $\left|P_{SNE}^{ND} - P_{SNE}^{NN}\right|$ for the northern well is 0.062; its maximum possible value is 1.0. $\left|P_{SNE}^{SD} - P_{SNE}^{SN}\right|$ for the southern well is 0.020. Once again, the northern well is superior.

Figure 5.4a shows P_{SNE} calculated over the model domain under the assumption that the proposed northern well does not detect contaminants. If the proposed northern well does detect contaminants the map is similar to Figure 5.2. Figure 5.4b shows P_{SNE} calculated over the model domain under the assumption that the proposed southern well does not detect contaminants. If the proposed southern well does detect contaminants the map is again very similar to Figure 5.2.

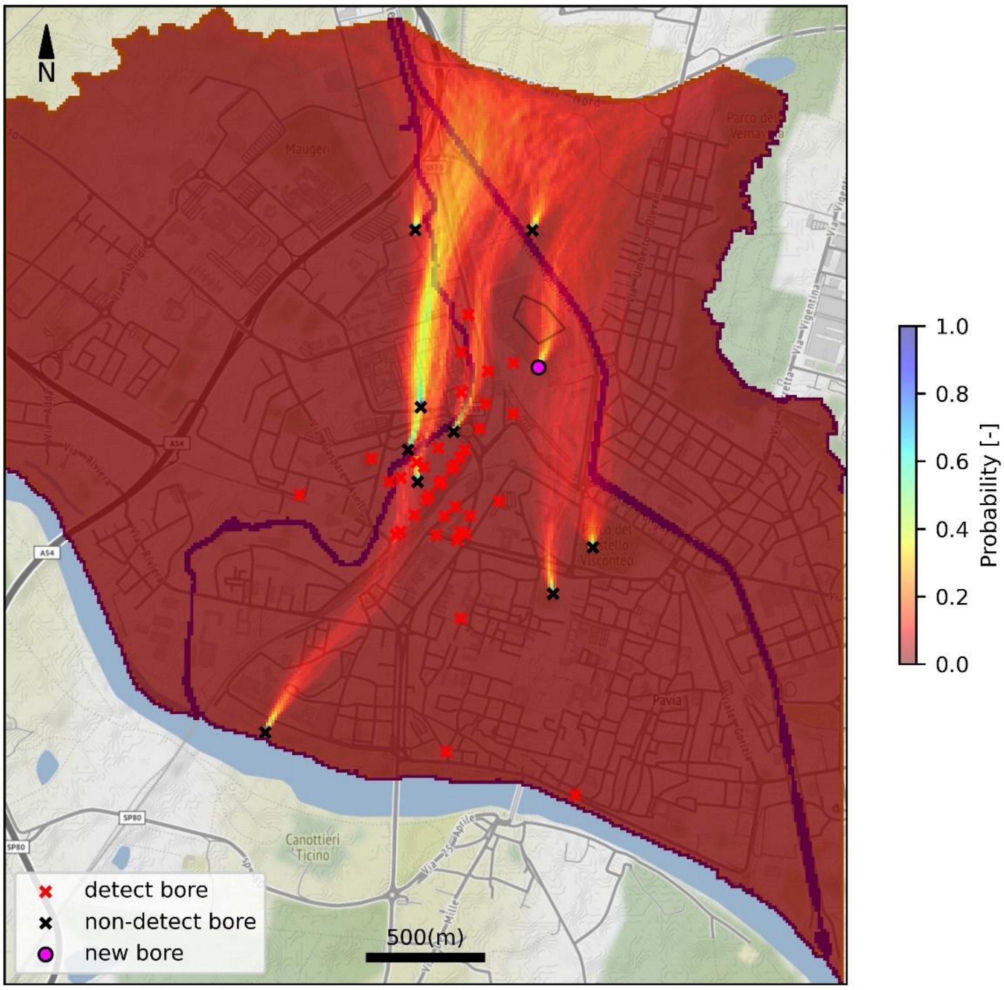

Figure 5.4a. Distribution of P_{SNE} under the assumption that the proposed northern well does not detect contaminants.

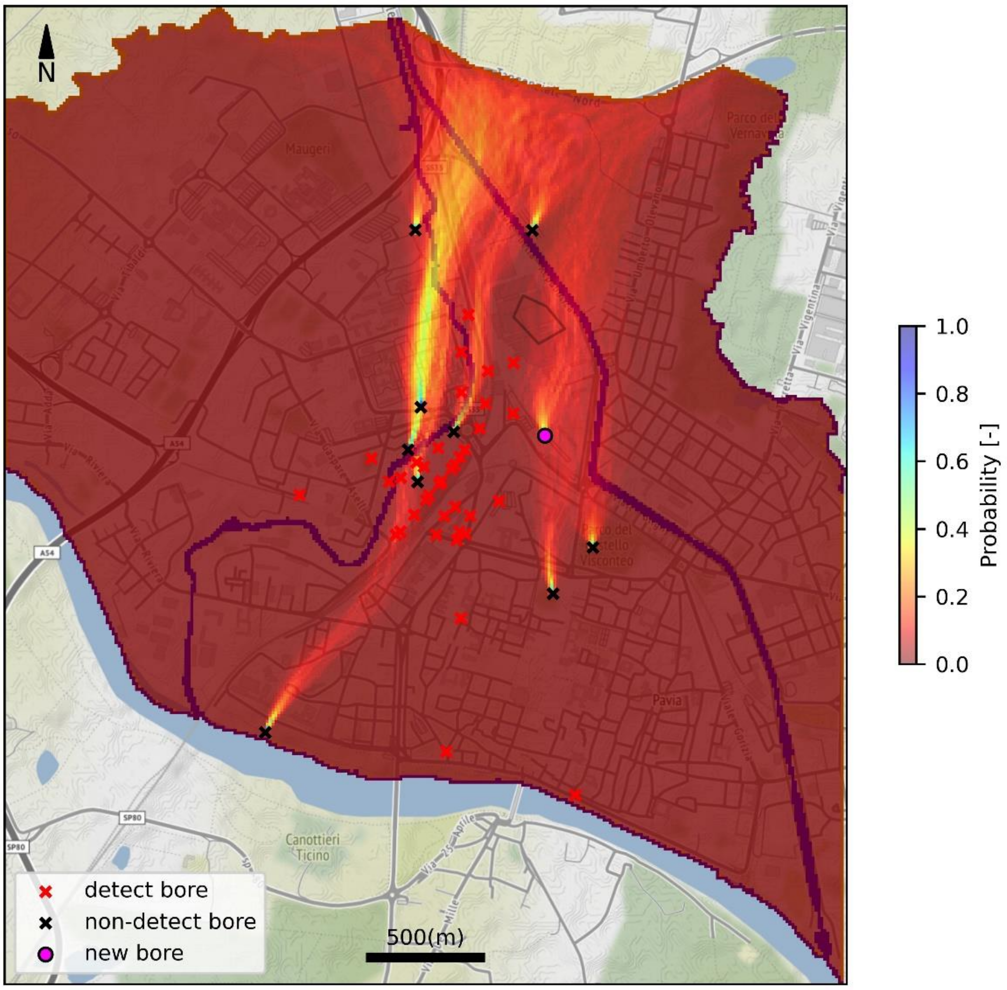

Figure 5.4b. Distribution of P_{SNE} under the assumption that the proposed southern well does not detect contaminants.

6. CONCLUSIONS

6.1 General

It is a recurrent theme of GMDSI webinars, tutorials and worked example reports that a modeller's ability to simulate subsurface processes is very limited. Another recurrent theme of GMDSI educational and technical products is that decision-support groundwater modelling is most productive when it is loyal to the scientific method. Fortunately, these two concepts are not incompatible. A modeller does not need to construct a digital replica of subsurface processes and properties in order to process groundwater data in ways that support the making of important groundwater management decisions.

Our knowledge of subsurface processes is vague. Conclusions that we can draw about its future and about its past are uncertain. It makes no sense to pretend otherwise. Processing of groundwater data must acknowledge the fact that the outcomes of this processing must be probabilistic. Management of groundwater systems can therefore be based on knowledge of the risks that management entails. Acknowledgement of uncertainty is also integral to experimental design, and hence to formulation of plans to acquire new data. Returns on investment in data acquisition rise with the ability of these new data to reduce the uncertainties of decision-critical predictions. This requires that they be processed in ways that extract the information that they hold, and direct that information to predictions of management interest.

The present worked example illustrates a new methodology for processing of groundwater contaminant data. The method is easy to apply. Its outcomes are probabilistic. These outcomes summarize all that can be known about a specific facet of groundwater behaviour given presently available information. They also provide a basis for maximising returns on investments in new data.

6.2 Particles

The modelling and data-processing methodology that is the subject of this GMDSI worked example report relies on the use of particles. Each particle can be visualised as carrying a small quantum of contaminant as it undergoes advective movement through the subsurface. (Note that random-walk particle methodologies support simulation of diffusive solute movement in addition to its advective movement; see, for example, Kinzelbach, 1988. However use of these methodologies is inappropriate for the current project. They add to the computational cost of using particles, while eliminating continuity of particle-derived model outputs with respect to model parameters.)

Computation of advective particle trajectories over long time frames is numerically cheap. This is especially the case if the groundwater flow field does not change over this time. It is also numerically stable. It can therefore be repeated many times for many different flow fields that are calculated using many different realizations of hydraulic properties.

A problem with the use of particles in an inverse problem setting is that they are granular, rather than continuous, entities. Solution of highly-parameterized inverse problems (through calibration, or through parameter ensembles) requires that model outputs that are matched to field observations be continuous with respect to model parameters. At first sight, this makes use of particles problematic where a history-matching dataset includes measurements of contaminant concentration.

The methodology that is presented in this report overcomes this problem. In doing so, it introduces the concept of a "halo of influence" that surrounds each particle track. The intensity of this halo diminishes in a continuous manner with distance from the trajectory of the particle according to a Gaussian decay function. This mimics the role of hydrodynamic dispersion while not explicitly simulating it. A modeller must assign values to variables that determine the width of this halo. Choice of these values can be somewhat arbitrary. However, it can be argued that the choice is no less arbitrary than that of choosing values for longitudinal and transverse dispersivity as is required for explicit simulation of hydrodynamic dispersion.

If an observation well falls within the zone of influence of a particle, it can contribute to the status of that particle. Because this contribution is calculated using a Gaussian function that is centred on the particle's path and decays continuously to zero with distance from the path, the influence of the observation well on the status of a particle is continuous. Therefore, if a particle's trajectory is altered in response to small modifications to local hydraulic conductivity, the change in the particle's status in response to these modifications is also slight (and differentiable). This continuous mode of information transfer from borehole data to a particle admits use of borehole-observed contaminant concentrations in model history-matching.

This is despite the fact that in the methodology that is described herein, borehole contaminant measurements are coded in a binary contaminant detection classification. This binary classification stipulates that an observation well is either within or without a contaminant plume. At first sight, this classification may seem to devalue the information content of borehole concentration measurements. However, the information content of these data are already devalued by the "hydrogeological noise" that accompanies them. It is also devalued by the suite of approximations that numerical solution of the advection-dispersion equation requires. It does not stretch the truth too far to suggest that a borehole measurement of contaminant concentration at a specific location at a specific time can do little more than inform a hydrogeologist whether, or not, a contaminant plume exists at that location at that time.

The methodology that we describe herein transfers particle status to location status. The location to which this status is transferred is the location at which the particle is introduced to the groundwater system. Because of the numerical cheapness of using particles, every cell within a model domain can be awarded a status. This status is related to the possibility that it hosts a contaminant source. By computing this possibility for many history-match-constrained realisations of random parameter fields, contaminant source probabilities can be mapped.

6.3 History-Matching

Between the observation that a well is within or without a contaminant plume, and the assignment of a contaminant source status to a particle's cell of origin, lies the problem of information transfer. In the methodology that we describe herein, information transfer is effected through the concept of particle inconsistency. A particle cannot be observed to carry a contaminant as it passes close to one observation well, and be observed not to carry a contaminant as it passes close to another observation well. This constraint must be imposed using a simulator in conjunction with data assimilation software such as PEST and PEST++.

Assimilation of contaminant concentration data is implemented by asking PEST/PEST++ to derive sets of hydraulic properties that maintain particle track consistency. This approach to contaminant data assimilation has two beneficial outcomes. Firstly, information-rich data are given a voice in model parameterization. This reduces the uncertainties of decision-critical model predictions. Secondly, when the status of a particle track is transferred to a particle source, only one status is transferred to that source for any given parameter field. When multiple parameter fields are employed to compute multiple instances of source point status, the same source point can be awarded different statuses. However, because these statuses are internally consistent for each parameter field, they can be used for construction of a source probability density function. This is achieved by averaging point statuses over many parameter fields. By contouring results over many points, probability maps can be constructed.

6.4 Probability Maps

The significance of a particle-status-derived probability map depends on the type of status from which the map is derived. Maps presented in the present report that are derived from particle detect statuses reveal the probability that a contaminant source can exist in any cell of the model domain, yet be undetected by the current monitoring network. In contrast, maps that are constructed from particle nondetect statuses reveal the probability that a contaminant source does not exist at any particular location within the model domain. Taken together, these two types of probability map depict the totality of information that can be gained from simulator-based processing of historical observations of groundwater elevation and contaminant concentrations.

Inferences that can be drawn from these maps are not conclusive, for they express probabilities. Nevertheless, when employed to support the making of a decision, the decision-maker is made aware of risks that he/she faces in choosing a particular course of management action. This is because simulator-based processing of all available data has revealed that which can be known about a system of interest. At the same time, it has revealed that which cannot be known about the system on the basis of currently available data.

6.5 Data Worth

One of the decisions with which a manager is often faced is that of whether he/she should invest in acquisition of extra data. Methodologies that are described in this report enable a direct connection to be made between an area of interest and locations where measurements of groundwater contaminant can be most effective in reducing uncertainties that pertain to that area. Once these data have been acquired, source status probability maps can be redrawn to reflect the new information. This process can be repeated as many times as desired.

Eventually, with acquisition of further head and concentration data, the history-matching process may need to be repeated. However, because the model is fast-running and numerically stable, this is not a difficult matter. Nor is the re-drawing of source probability maps.

6.6 Modelling Philosophy

As is discussed above, we adopt as our guide for decision-support modelling implementation of the scientific method. In accordance with principles set out by Doherty and Moore (2021), our strategy for its implementation is that of structural simplicity and parametric complexity. Structural simplicity enables numerical simulation that is fast, stable and prediction-focussed. Parametric complexity supports the free flow of information from data wherein it resides to the receptacles that a model provides for this information; these are its parameters. This information can then be directed to decision-critical predictions in order to reduce their uncertainties. The ramifications of information insufficiency, namely predictive uncertainty, can also be assessed.

We find the outcomes of the present study particularly pleasing as they are able to demonstrate in two informative maps the decision-salient outcomes of model-based data processing. These outcomes are both probabilistic and definitive. They are probabilistic because they expose the uncertainties that prevail after decision-pertinent processing of all available data has taken place. They are definitive because they define a clear path towards reduction of these uncertainties through targeted acquisition of further data.

7. REFERENCES

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APPENDIX A: SOFTWARE

The table provided below lists programs that were used to implement analyses that are documented in this worked example report. Except for MODFLOW 6 and MODPATH 7, they all belong to the PEST/PEST++ and PEST-support utility suites. PEST-suite software is downloadable from the PEST web site at: http://www.pesthomepage.org. PEST++ programs are downloadable from https://github.com/usgs/pestpp

The following table does not include Python code that was used for model and PEST/PEST++ setup. Much of this code belongs to the FloPy and PyEMU packages. These are downloadable from https://github.com/modflowpy/flopy and https://pypi.org/project/pyemu respectively. A small amount of Python code was self-written. This was developed and implemented for convenience; it is not fundamental to any of the work that is discussed in this report. Note also that model setup could just as easily have been undertaken using a graphical user interface. PEST setup could just as easily have been undertaken using members of the PEST Groundwater Utility Suite.

As is discussed in the body of this report, we used MODFLOW 6 for simulation and MODPATH 7 for computation of particle paths. MODFLOW-USG and mod-PATH3DU comprise viable alternatives. The PEST Groundwater Utility Suite contains many programs for post-processing of MODFLOW-USG and mod-PATH3DU output files. The latter can be easily modified to comprise replacements for some of the programs listed below.

Program	**Role**
MF6MOD2OBS	Reads a binary system state file written by MODFLOW 6; often this file contains model-calculated heads. Undertakes temporal/spatial interpolation to the times and locations of borehole head observations. This is a member of the PEST Groundwater Utility Suite.
MODFLOW 6	A groundwater flow simulator provided by the USGS.
MODPATH 7	A USGS-produced particle tracking post-processor for programs of the MODFLOW suite.
MP72MIF MP72MIF1 MP72MIF2	Translate MODPATH 7 particle outputs to a format that can be readily imported into a Geographical Information System (GIS). These are members of the PEST Groundwater Utility Suite.
MP72VTK	Translates MODPATH 7 particle outputs to a format that allows importation into a visualisation/display platform such as PARAVIEW. MP72VTK belongs to the PEST Groundwater Utility Suite.
MP7DIST2PATH	Reads a *pathline* file produced by MODPATH 7. Evaluates the distance of closest approach of a series of particles to a series of observation wells. This is a member of the PEST Groundwater Utility Suite.
PCDETACCUM	Accumulates PCDETECT results over many parameter realisations and complementary model runs to generated contaminant source detect and nondetect probability distributions. These can be related to contaminant source probabilities. This is a member of the PEST Groundwater Utility Suite.

PCDETECT	Reads a MP7DIST2PATH output file. Confers a detect, nondetect or inconsistency status on all particles cited therein. This is a member of the PEST Groundwater Utility Suite.
PLPROC	This is supplied with the PEST suite. It is used for pilot point parameterisation of a model domain.
PEST_HP	A member of the PEST suite. PEST_HP undertakes highly-parameterized, regularised inversion.
PESTPP-IES	An iterative ensemble smoother supplied with the PEST++ suite.

Table A1. Programs used to undertake work that is documented in the present report.

gmdsi

Groundwater Modelling
Decision Support Initiative

gmdsi.org