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Accessible probabilistic modeling of wellhead protection areas for small and medium-sized water supplies

Nadine Gärtner^{1*} , Maryam Zamzami² and Andreas Lindhe¹

*Correspondence:

Nadine Gärtner
gaertner.nadine@gmail.com

¹Department of Architecture and Civil Engineering, Division of Geology and Geotechnics, Chalmers University of Technology, 41296 Gothenburg, Sweden

²Department of Sustainable Development, Environmental Science and Engineering (SEED), KTH Royal Institute of Technology, 100 44 Stockholm, Sweden

Abstract

Groundwater supplies nearly half of the global population with drinking water but faces increasing contamination risks. Delineating Wellhead Protection Areas (WHPAs) is essential for safeguarding groundwater quality, yet uncertainty in subsurface parameters complicates this process. Here we present a practical probabilistic workflow combining Monte Carlo simulation with the Analytic Element Method, implemented within an open-source Python framework. This method generates an ensemble of capture-zone realizations by incorporating parameter uncertainties through repeated simulations, with results visualized via GIS tools and summarized as percentile-based WHPA envelopes. Applied to a Swedish aquifer case study, the approach aligns well with deterministic numerical models while better capturing variability. In rural and semi-rural settings, the workflow can serve as a first screening step by showing how uncertainty changes the extent of the WHPA and which surrounding land uses may be affected under different precautionary delineations. By making uncertainty-aware WHPA delineation accessible to small and medium-sized water suppliers with limited resources, this method supports improved groundwater protection and aligns with emerging legislative requirements for risk-based water source management.

Keywords Probabilistic wellhead protection areas, Analytic element method, Groundwater protection, Small supplies, Small and medium-sized water supplies

1 Introduction

Approximately 50% of the world's drinking water is sourced from groundwater [1]. Despite its subsurface location, groundwater is increasingly threatened by pollution, overuse, competing land uses, and changes in hydrogeological and hydrochemical conditions driven by climate change [2–4]. While some groundwater sources benefit from a natural protective layer, many are vulnerable, with land use posing significant risks. Once contaminated, aquifers are difficult to remediate, making their protection essential for maintaining a consistent supply of potable water [5].



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One key strategy for groundwater protection is the establishment of Wellhead Protection Areas (WHPAs), which are designed to safeguard drinking water sources by controlling land use in areas contributing to wells. WHPAs are commonly delineated based on time-of-travel criteria, identifying regions from which water flows to a well within a specified time frame (e.g., 100 days, 365 days, 5 years) [6, 7]. A range of methods is available for delineating WHPAs, from analytical approaches to numerical models. Analytical methods calculate the capture radius of the well based on a specified travel time [6]. These methods often yield closed-form solutions to specific groundwater flow problems, relying on mathematical equations and idealized assumptions. Numerical methods, by contrast, are implemented in software packages such as MODFLOW [8], FEFLOW [9], HydroGeoSphere [10], and CATHY [11]. These models provide grid-based solutions for groundwater flow and transport.

Accurate delineation of WHPAs is critical, as these zones often come with land-use restrictions and may require compensation for affected stakeholders. However, accurately delineating WHPAs is complex due to the inherent uncertainty in subsurface parameters. Studies, such as Bhatt [12], have shown that deterministic approaches, which rely on fixed parameter values, can produce overly optimistic delineations that do not adequately reflect the uncertainty present in aquifer systems. Raymond et al. [13] demonstrated that simple volumetric methods are often insufficient to properly delineate WHPAs and address the uncertainties inherent in aquifers.

Recent legislative changes in countries such as Sweden have acknowledged these limitations and are shifting towards risk-based approaches that explicitly incorporate uncertainty into WHPA delineation [14]. Despite the availability of advanced numerical models capable of integrating uncertainty, such as MODFLOW with GMS [15], their complexity, data demands, and computational requirements make them impractical for many practitioners, particularly those working with small or medium-sized water supplies. As a result, many practitioners revert to simpler, more conventional modelling methods that often neglect uncertainty [16].

The Analytic Element Method (AEM) offers a promising alternative for WHPA delineation. Pioneered by Strack, AEM is a groundwater modeling technique that simulates groundwater flow by superimposing elementary analytical solutions, such as line sources or sinks, to represent complex aquifer configurations in two or three dimensions [17–19]. This approach allows for efficient and adaptable analysis of hydrogeological behavior, balancing the simplicity of analytical methods with the flexibility of numerical approaches. When combined with Monte Carlo Simulation (MCS) which assesses uncertainty and sensitivity by repeatedly sampling input parameters from probability distributions [20], AEM can generate probabilistic delineations that explicitly incorporate parameter uncertainty into WHPA delineation. MCS is a well-established and practical approach to address the inherent uncertainties associated with groundwater modelling [21]. In particular, the combination of MCS and the AEM framework is a valuable and practical approach for addressing the inherent uncertainties associated with WHPA delineation.

Various software options are available for calculating Wellhead Protection Areas using the Analytic Element Method [22], but none has so far included easy-to-use uncertainties into the available software. A widely used software is WhAEM, developed by the U.S. Environmental Protection Agency [23]. WhAEM features a user-friendly graphical

interface and is based on the original C code developed by Strack. However, it is important to note that WhAEM does not account for parameter uncertainties, and its source code is inaccessible for customization. In recent years, Bakker [24] introduced an open-source AEM package called TTim (later: TimML), written in the Python programming language. Its open-source nature and Python foundation provide the flexibility to modify the code and incorporate additional packages, enabling the inclusion of Monte Carlo simulations for a more comprehensive assessment of uncertainties.

This study develops a probabilistic WHPA delineation approach by integrating Monte Carlo Simulation with the Analytic Element Method and evaluates its performance against a numerical modeling benchmark. Using the open-source Python-based TimML package [24], we implemented a dedicated Monte Carlo component. We developed a pre-processor to define uncertain inputs as probability distributions and a post-processor to visualize outputs in a GIS environment. The workflow is designed to be usable for small and medium-sized water supplies and supports emerging requirements to consider risk and uncertainty in WHPA delineation. We demonstrate the approach for the Varnum aquifer in Sweden and discuss how the resulting probabilistic delineations can support groundwater protection planning.

2 Methodology

2.1 Overview

The applied method is based on groundwater flow modeling and particle tracking with consideration of uncertainties in input parameters. The conceptual diagram of the coupled Analytic Element Method (AEM) and Monte Carlo Simulation is illustrated in Fig. 1. The WHPA is defined as the area where particles can move within groundwater flow when tracking their path lines in a backward direction. The U.S. EPA has introduced five criteria for WHPA delineation, including distance, drawdown, time of travel,

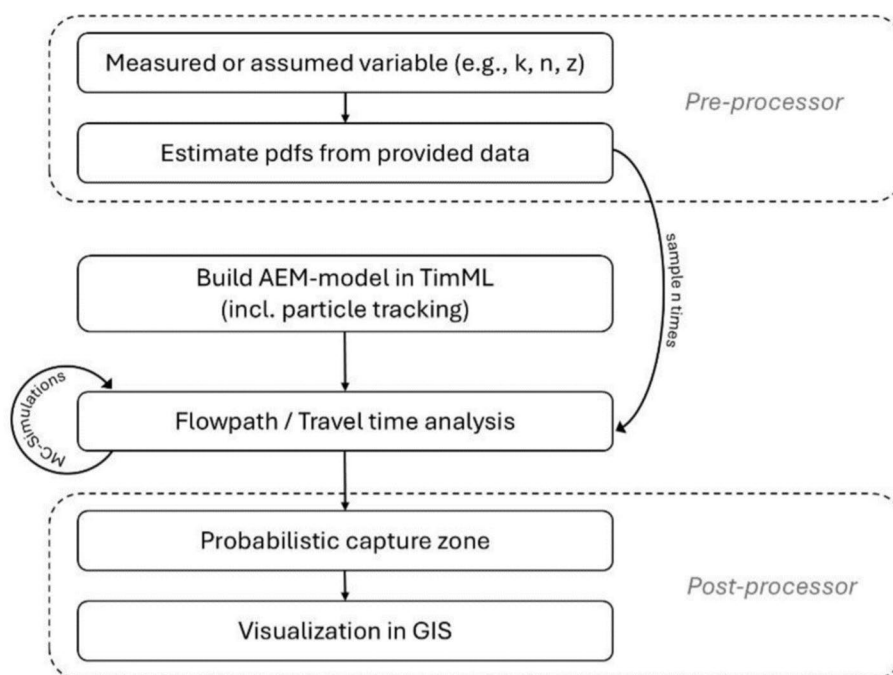


Fig. 1 Workflow for probabilistic capture zone analysis, involving pre-processing of input variables, AEM modeling and flowpath analysis in TimML, and GIS-based visualization of results

flow boundaries, and assimilative capability, which can be applied individually or in combination [6, 7]. The time-of-travel criterion is widely used in WHPA delineation and was also used in this analysis. Following previous Swedish guidance, travel times of 100 days (primary zone) and 365 days (secondary zone) are used [25].

The workflow is implemented in Python and provided as three Jupyter notebooks in the supplementary material: (S1) pre-processing and definition of uncertainty distributions, (S2) Monte Carlo sampling and repeated TimML runs, and (S3) GIS-based post-processing and visualization.

2.2 Groundwater model and particle tracking

The analytic element method (AEM) represents groundwater flow by superimposing analytical solutions (analytic elements) associated with conceptual hydrogeological features such as wells, boundaries, and line sinks [17, 18, 26–28]. Because the method does not require spatial discretization of the domain, it avoids grid-related artefacts and allows model inputs to be specified directly in terms of hydrogeological features and boundary conditions.

WHPAs are delineated using TimML 6.4.1 [29], an open-access modelling framework written in Python and Fortran [24, 30, 31]. TimML solves the governing groundwater flow equation under the adopted conceptual assumptions and computes pathlines and travel times through particle tracking. In this paper, particle pathlines are generated for each Monte Carlo realization, and the ensemble of resulting pathlines forms the basis for probabilistic WHPA delineation. For further details on AEM, we refer the reader to [17,18] and to the recent book *Analytical Groundwater Modeling* by Bakker and Post [26].

2.3 Uncertainty representation and parameter distributions

In this paper, “uncertainty” refers to both (i) aleatory uncertainty arising from natural variability, for example spatial heterogeneity in hydraulic conductivity, and (ii) epistemic uncertainty arising from limited measurements and imperfect knowledge of site conditions. The modelling approach can represent heterogeneity only to the extent that it is included in the conceptual model. In the present case study, the aquifer is represented as a single hydrogeological unit with effective properties (homogeneous, potentially anisotropic). Uncertainty is therefore implemented by assigning probability distributions to representative parameter values and sampling these values across Monte Carlo realizations. This primarily captures epistemic uncertainty in the effective parameterization, while variability in the available measurements is reflected indirectly through the spread of the fitted distributions. A potential extension is to subdivide the aquifer into multiple zones (inhomogeneity units) and assign separate uncertain properties to each zone, which would enable a more explicit representation of heterogeneity at the chosen zonal scale. This extension is not implemented here.

Three parameters are treated as uncertain because they are often poorly constrained and strongly influence travel-time based capture zones: hydraulic conductivity (K), aquifer thickness (H), and effective porosity (n_e). Given limited data, aquifer thickness and porosity are represented by truncated normal distributions bounded by physically plausible minimum and maximum values. The standard deviations are defined so that these bounds correspond approximately to the mean ± 3 standard deviations, allowing

broad but physically realistic sampling while preventing implausible values outside the specified range. Hydraulic conductivity is commonly represented as lognormal in hydrogeological applications because it is strictly positive and often spans several orders of magnitude [32]. We therefore evaluate whether the observed data is consistent with a lognormal assumption using Q–Q plots and the Shapiro–Wilk test on $\ln(K)$. Based on this assessment, K is represented as lognormally distributed. Parameters of the selected distributions (mean and standard deviation, or log-space equivalents) are estimated from the available measurements. Where a conservative estimate of the mean is required, an upper confidence limit of the mean (UCLM) is computed using a t -distribution. For normally distributed data:

$$UCLM = \bar{X} + t \cdot ppf\left(1 - \frac{\alpha}{2}, N - 1\right) \cdot \frac{s}{\sqrt{N}} \quad (1)$$

For lognormally distributed data, a Cox-modified method is applied in log space [33]:

$$UCLM = \bar{Y} + \frac{\bar{s}^2}{2} + t \cdot ppf\left(1 - \frac{\alpha}{2}, N - 1\right) \cdot \sqrt{\frac{\bar{s}^2}{N} + \frac{\bar{s}^4}{2(N - 1)}} \quad (2)$$

where $\bar{X}$ and s are the sample mean and standard deviation, N is the number of observations, and $\bar{Y}$ and $\bar{s}$ are the mean and standard deviation of the natural-log-transformed data.

$$\sigma = \frac{UCLM - \bar{X}}{z} \quad (3)$$

We use Eq. 3 to derive the population standard deviation used for Monte Carlo sampling from the estimated confidence limit of the mean.

2.4 Monte Carlo coupling and repeated TimML runs

Monte Carlo simulation is used to propagate parameter uncertainty into WHPA delineation. For each realization, a unique parameter set (K, H, n_e) is sampled from the defined probability distributions and assigned to the TimML model. The model is then run and reverse pathlines are generated for the specified travel times. This produces one plausible WHPA realization given the sampled parameter values. Repeating the procedure yields an ensemble of equally plausible WHPA realizations. Latin Hypercube Sampling could be used to reduce the required number of runs, but was not necessary here due to practical runtimes for the present case based on available hardware.

2.5 Post-processing and probabilistic WHPAs

After each TimML run, reverse particle tracking yields a set of pathlines (for example, 20 pathlines per realization) for the selected travel times. Across all Monte Carlo realizations, these pathlines provide an ensemble of equally plausible capture-zone representations rather than a single deterministic boundary. The percentiles reported in the following are derived from this output ensemble, not from the input parameter distributions themselves. In other words, the means and standard deviations define how the uncertain inputs are sampled, whereas the 50th, 75th, 95th, and 99th percentiles are used to summarise the resulting spread in simulated pathline distances and WHPA extent. In practice, the particle locations along these pathlines are pooled across realizations,

and the selected percentile is applied to their distance from the pumping well across the Monte Carlo ensemble to define the WHPA envelope. Probabilistic WHPAs are derived from this ensemble using percentile-based thresholds, where the selected percentile reflects a chosen level of conservatism. The choice of percentile is user-defined and may depend on risk preference and the importance of the groundwater resource; here, the 50th, 75th, 95th, and 99th percentiles are used to illustrate progressively more conservative delineations. This representation was chosen because it provides a compact and practical way to summarise the ensemble for planning purposes, from more central to more precautionary delineations. In this implementation, smaller percentiles yield larger, more precautionary WHPAs because only points beyond the percentile distance are excluded before polygon construction. For example, at the 99th percentile, only the most extreme 1% of pathline distances extend beyond the applied threshold.

To compute percentile-based boundaries, distances from the pumping well to particle locations along the pathlines are calculated for all realizations. Two general approaches are possible: (1) calculating percentiles using the full set of pathline points, or (2) using only the maximum distance per realization. Approaches based on pathline envelopes have also been used to distinguish “confident” and “unconfident” zones [34]. In this study, percentiles are computed from the full pathline dataset to use all available spatial information from each realization. For each percentile, points exceeding the corresponding distance threshold are excluded, and the remaining points are converted to a polygon using a convex hull algorithm (the smallest convex polygon enclosing the selected points). The resulting WHPA polygons are georeferenced in SWEREF 99 for GIS visualization and comparison with existing delineations.

3 Case study site

3.1 Site description

The Varnum aquifer is located in southwest Sweden, within the municipality of Borås (Fig. 2). The area is predominantly rural, with a landscape characterized by farmland interspersed with forests. Numerous lakes and streams are present throughout the region. The aquifer is situated in a valley with an elevation of approximately 170–175 m above sea level (m.a.s.l.), surrounded by higher terrain ranging from 200 to 270 m.a.s.l. The aquifer is unconfined and primarily composed of glaciofluvial delta deposits, which



Fig. 2 Locator map of the Varnum study area. The left panel shows the location of the study area in Sweden. The middle panel provides a detailed view of the case study area, highlighting the well location (black point). The right panel presents the Varnum aquifer boundary overlaid on the same background, showing key hydrological features and spatial extent

are part of the Rångedala esker. This esker runs north-south along a valley formed by a fracture zone in the same direction.

The aquifer also includes some deposits of ice lake sediment and widens where it intersects an east-west fracture zone, resulting in greater deposit thickness in this area. The Varnum aquifer spans an area of about 3 km², with deposit thickness varying between 20 and 55 m. Figure 3 provides a typical cross-sectional profile of the aquifer, illustrating the stratification of geological layers along a west-east transect. Fine sand forms the uppermost layer, followed by medium to coarse sand, with bedrock as the lowermost unit. This type of aquifer, characterized by its distinct geological and hydrogeological features and associated land use, is typical for Sweden and can be found across the country. These aquifers, especially if unconfined and not overlain by low-permeability deposits, are particularly vulnerable to contamination due to their shallow depth to the water table.

3.2 Conceptual model

The study site is represented using analytic elements to describe the hydrogeological conditions (Fig. 4). The aquifer is modeled as a single layer with uniform hydraulic conductivity, underlain by impermeable bedrock that outcrops in the eastern part of the site. The bedrock depth is relatively consistent across the area and is assumed to be at 155 m.a.s.l. The aquifer is bounded by shallow lakes and rivers, which also serve as the model boundaries. Groundwater flow is unconfined and predominantly horizontal, making the model suitable for the Dupuit-Forchheimer approximation and compatible with the TimML modeling framework. Historical head measurements collected over 10 years indicate that the groundwater table has remained stable throughout the aquifer. Based on this observation, the flow is modeled under steady-state conditions.

4 Results

4.1 Probability density functions for uncertain input parameters

The pre-processing step produces the probability density functions (PDFs) used to represent uncertainty in the hydrogeological inputs for the Varnum case study. Table 1 summarizes the deterministic inputs (pumping rate and recharge) and the uncertain inputs (hydraulic conductivity K , saturated thickness H , and effective porosity n_e), including the adopted distribution types and parameterization.

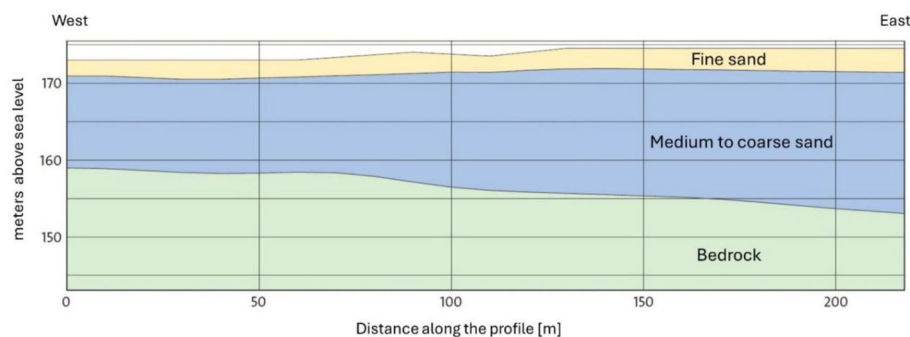


Fig. 3 Typical cross-sectional profile of the aquifer along a west-east transect, showing stratification of geological layers. The profile consists of fine sand (yellow) at the top, underlain by medium to coarse sand (blue), with bedrock (green) forming the lowermost layer. Elevation is measured in meters above sea level, and the horizontal axis indicates the distance along the profile in meters. Modified after [35]

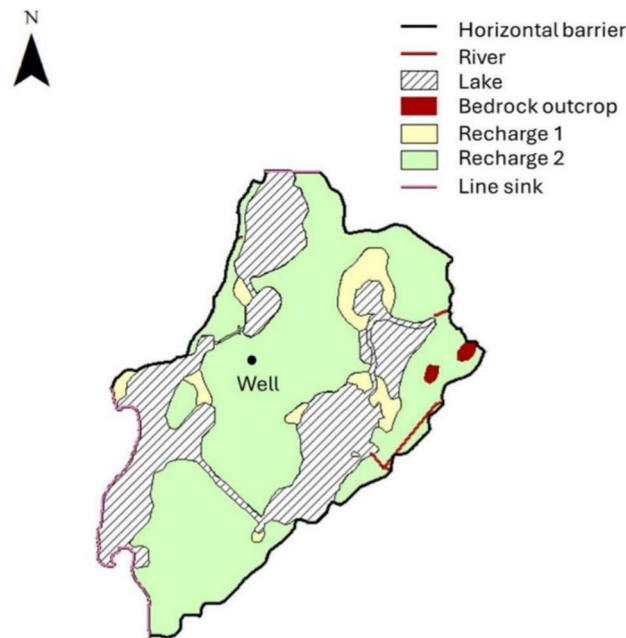


Fig. 4 Map of analytic elements in the Varnum region, showing recharge areas, bedrock outcrops, horizontal barriers, rivers, lakes, and the central well location. These elements define the flow boundaries and controls within the analytical model

Table 1 Hydrogeological inputs used for the Varnum pumping site

Category	Variable	Unit	Distribution	Parameters/summary
Deterministic	Pumping rate	L/s	Fixed	50
Deterministic	Recharge rate	mm/year	Fixed	549
Uncertain	Saturated thickness (H)	m	Truncated normal	Bounds [20, 55], mean 37.5, SD 5.83
Uncertain	Effective porosity (n_e)	fraction	Truncated normal	Bounds [0.15, 0.25], mean 0.20, SD 0.0167
Uncertain	Hydraulic conductivity (K)	m/day	Lognormal	Observed range 0.049 to 492.48, mean 30.80 ($n=70$); $\ln(K)$ normality: $W=0.974$, $p=0.161$

Deterministic inputs are fixed values. Uncertain inputs are represented by probability distributions used to sample parameter values for probabilistic WHPA delineation

Hydraulic conductivity is compiled from 70 Hazen-based estimates derived from grain-size information and converted to the TimML unit of m/day. The observed dataset spans values from 0.049 to 492.48 m/day with a mean of 30.80 m/day (Table 1). Figure 5 compares normal and lognormal assumptions for K . The Q–Q plot indicates that untransformed K deviates from normality, whereas $\ln(K)$ aligns closely with normal quantiles. Consistent with this visual assessment, a Shapiro-Wilk test applied to $\ln(K)$ indicates no statistically significant deviation from normality ($W = 0.974$, $p = 0.161$, $n = 70$). Hydraulic conductivity was therefore represented as lognormally distributed in subsequent simulations.

Saturated thickness and effective porosity are represented by truncated normal distributions bounded by physically plausible limits (Table 1). Saturated thickness is bounded between 20 and 55 m (mean 37.5 m), and effective porosity between 0.15 and 0.25 (mean 0.20). Because the aquifer is represented as a single hydrogeological unit in the AEM model, each TimML realization uses one representative (spatially uniform) value for

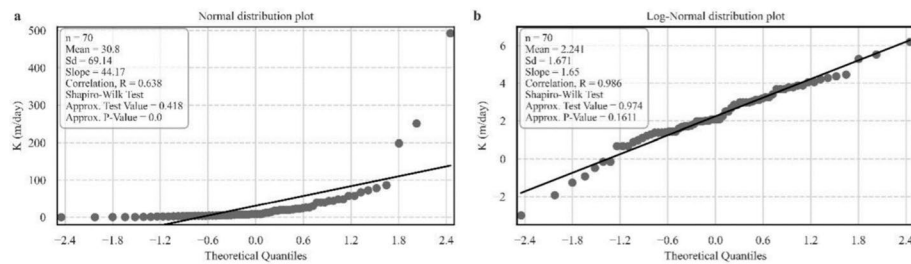


Fig. 5 Goodness-of-fit analysis for hydraulic conductivity data. **a** Quantile-quantile (Q–Q) plot for the normal distribution and **b** Q–Q plot for the log-normal distribution. The plots compare observed quantiles with theoretical quantiles for each distribution. The variables in the figure include sample size N , mean and standard deviation of the dataset, the slope of the best-fit line, correlation coefficient R , and results of the Shapiro-Wilk test (test statistic and p-value)

each uncertain parameter. Accordingly, the Monte Carlo ensemble reflects uncertainty in the effective parameterization of the conceptual unit, rather than explicitly resolving spatial heterogeneity within the aquifer.

4.2 Benchmarking against a numerical model

We benchmark the AEM-based delineations against an existing deterministic numerical model for the Varnum site (Fig. 6). The numerical model was previously developed, calibrated, and approved by the Municipality of Borås, and its original analysis included reverse particle tracking for a 100-day travel time. For this study, the 100-day pathlines from the numerical model are obtained and digitized to enable a spatial comparison.

The digitized numerical-model pathlines are then compared with the probabilistic AEM results for the same travel time. Overall, the numerical-model pathlines fall within the central part of the probabilistic envelope and are most consistent with the 75th to 50th percentile delineations derived from the Monte Carlo ensemble. This is consistent with the interpretation that a deterministic parameter set represents one plausible realization near the centre of the assumed distributions.

4.3 Probabilistic wellhead protection areas

Probabilistic WHPAs are derived from the ensemble of reverse particle-tracking results obtained across all Monte Carlo realizations for a 100-day travel time. Rather than producing a single deterministic capture-zone boundary, the repeated simulations yield many equally plausible pathline sets that reflect uncertainty in the sampled input parameters. To summarize this ensemble, percentile-based WHPA envelopes are delineated (P50 to P99). Higher percentiles represent more central delineations of the ensemble, while lower percentiles represent progressively more conservative envelopes. The resulting WHPA polygons for the 50th, 75th, 95th, and 99th percentiles are exported as georeferenced GIS layers for visualization and further analysis (Fig. 7).

The results show a strong expansion of WHPA extent as more conservative percentiles are selected. The 50th percentile WHPA covers 32,260 m² (3.23 ha) and is concentrated around the well. At the 75th percentile, the WHPA increases to 155,980 m² (15.60 ha) and intersects a broader range of land uses, including agricultural and residential areas, as well as locations that may warrant additional consideration such as cemeteries. Cemeteries have been discussed in the literature as potential sources of groundwater contamination through leaching processes [36]. At the 95th and 99th percentiles, the WHPA

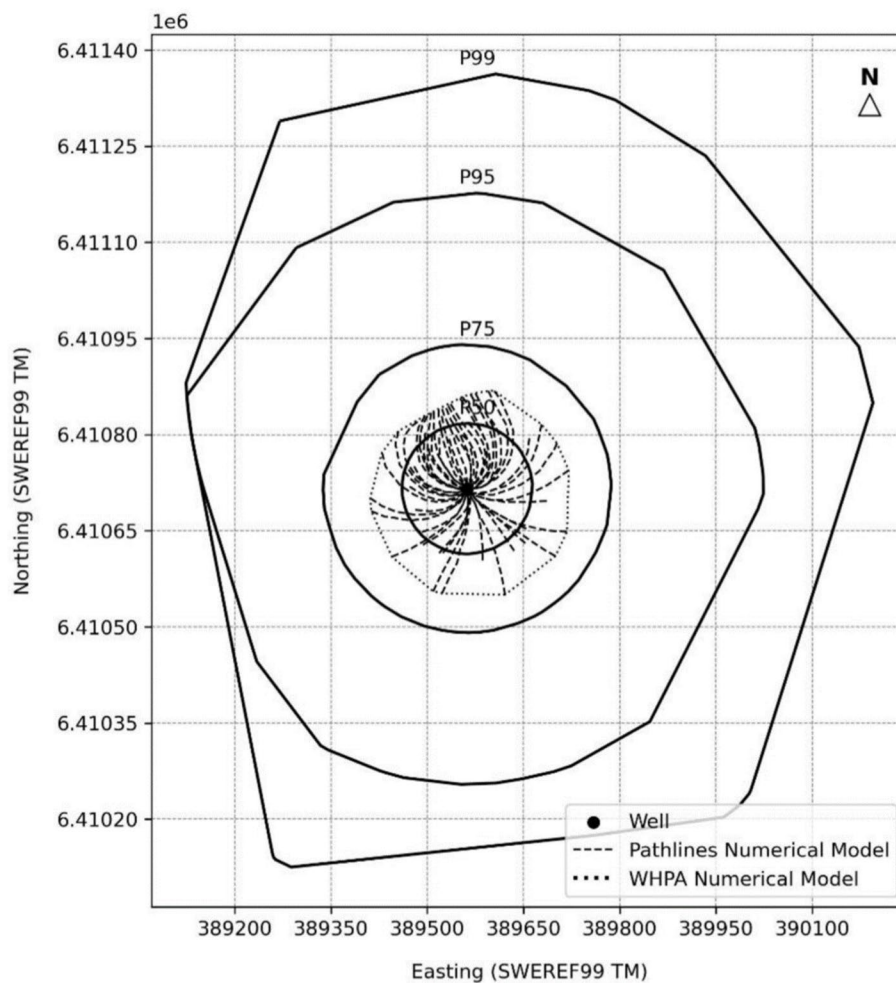


Fig. 6 Percentile-based WHPA envelopes derived from the Monte Carlo ensemble (50th, 75th, 95th, and 99th percentiles) for a 100-day travel time. Digitized 100-day reverse pathlines from the deterministic numerical model are overlaid for comparison and fall within the central part of the ensemble, most consistent with the 25th to 50th percentile envelopes

expands further to 617,137 m² (61.71 ha) and 1,020,975 m² (102.10 ha), respectively, and includes additional land-cover types such as peat bogs (Table 2). Peatland environments can be associated with elevated dissolved organic carbon (DOC), which may influence groundwater quality and treatment requirements, particularly under changing land use or climate conditions.

Table 2 summarizes the distribution of land-use categories within the percentile-based WHPAs. Agricultural and non-irrigated arable land contribute substantially across all percentiles, reflecting the land-use setting of the pumping site. As the WHPA envelope expands at higher percentiles, overlaps with residential areas become more likely (Fig. 7), which can increase the range of potential contaminant sources (e.g., septic systems, household chemicals, and urban runoff). From a planning perspective, these percentile-based WHPA envelopes provide a practical way to explore how uncertainty affects which land uses fall within the protection area and how precautionary delineations may lead to broader land-use considerations.

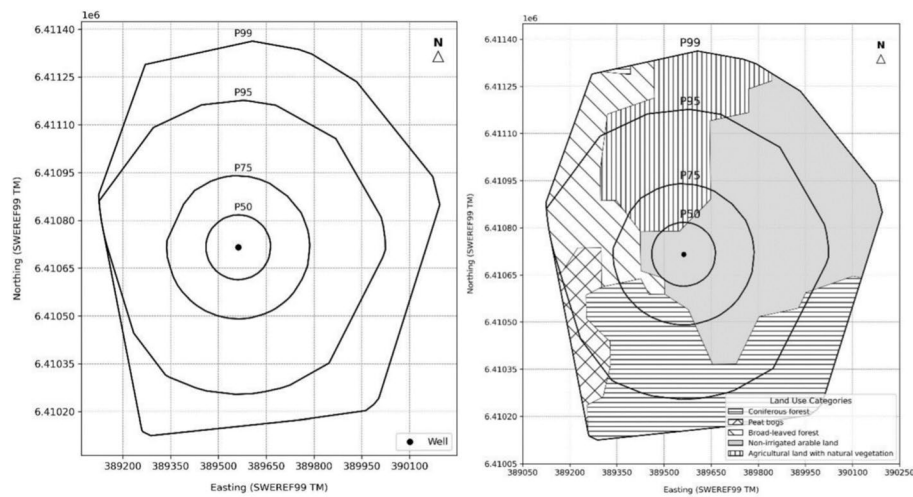


Fig. 7 Left: Percentile-based WHPA envelopes derived from the Monte Carlo ensemble for a 100-day travel time (50th, 75th, 95th, and 99th percentiles). Right: Land use categories intersecting the WHPA envelopes at each percentile

Table 2 Distribution of land use categories within percentile-based wellhead protection areas (WHPAs) at different percentiles

Percentile	Total Area	Agricultu- ral land	Broad- leaved forest	Coniferous forest	Non-irrigated arable land	Peat bogs
50	32,260	1322	17	0	30,921	0
75	155,980	28,192	18,200	15,934	93,654	0
95	617,137	113,173	77,814	140,375	256,377	29,398
95	1,020,975	179,575	124,777	287,277	380,332	49,014

The table presents the total area (m²) and the contributions of specific land use types, including agricultural land, broad-leaved forest, coniferous forest, non-irrigated arable land, and peat bogs, for the 50th, 75th, 95th, and 99th percentiles

5 Discussion

5.1 Case study outcomes

This study presents a probabilistic WHPA delineation workflow that couples Monte Carlo sampling of uncertain input parameters with an Analytic Element Method (AEM) model and reverse particle tracking. Using the Varum aquifer as a case study, the workflow generates an ensemble of WHPA realizations and summarizes them as percentile-based WHPA envelopes (50th, 75th, 95th, and 99th), providing a transparent way to explore how uncertainty in parameter values affects delineation outcomes.

Comparison with an existing deterministic numerical model showed that the numerical-model pathlines fall within the central part of the AEM-based ensemble, most consistent with the 50th to 75th percentile envelopes. This supports the interpretation that a deterministic parameter set represents one plausible outcome near the centre of the assumed input distributions. At the same time, the percentile-based envelopes illustrate that more conservative delineations can extend substantially beyond a central estimate, depending on uncertainty in inputs such as hydraulic conductivity, thickness, and effective porosity.

Across the case study, WHPA extent increases markedly as more conservative percentiles are selected. In the Results, the WHPA area increases from 32,260 m² at the 50th percentile to 155,980 m² at the 75th percentile, 617,137 m² at the 95th percentile, and

1,020,975 m² at the 99th percentile (Table 2). Practically, this means that progressively larger areas would fall within the protection zone and would need to be considered in planning, monitoring, and potential land-use restrictions. The results therefore highlight an inherent trade-off between precaution and the extent of constraints placed on surrounding land uses. As noted by Sousa et al. [37], the safest decision under uncertainty may differ from an “optimal” decision in a statistical sense. In the Varum case, adopting very conservative envelopes would bring larger areas of agricultural land, forest, and peatland environments into the protection zone, which could imply broader management measures (for example, restrictions on fertilizer application) even when those areas are only included under conservative uncertainty assumptions. It should be noted that final WHPA zoning in practice is often adjusted to follow roads, parcel boundaries, and other administrative constraints. Such alignment can further expand the final protected area beyond the hydrogeologically derived percentile envelope, so the choice of percentile can have an amplified effect on the final zoning extent.

5.2 Limitations

The proposed probabilistic WHPA workflow is designed as a practical way to incorporate parameter uncertainty into WHPA delineation for small and medium-sized supplies. The main limitations therefore reflect the chosen level of conceptual detail and the type of data that is typically available at such sites.

First, the results depend on the probability distributions assigned to uncertain inputs. Where measurements are sparse or based on indirect estimates (for example, Hazen-based hydraulic conductivity values), the resulting PDFs should be interpreted as plausible representations of uncertainty rather than definitive characterizations of the aquifer. This is not unique to the present workflow. It also applies to standard deterministic delineations, where the same limited information is often condensed into a single “best estimate” parameter set. The added value here is that uncertainty is made explicit and can be explored transparently. In the present study, uncertain parameters were sampled independently. This was a deliberate simplification to keep the workflow transparent and straightforward to interpret for small and medium-sized supplies. Where sufficient site-specific data are available, correlated sampling could be introduced to avoid jointly unlikely parameter combinations and to test how strongly the outer percentile-based WHPAs depend on this assumption.

Second, the Varum case study represents the aquifer as a single hydrogeological unit with spatially uniform (but uncertain) properties in each realization. This is a deliberate choice aligned with common practice for small and medium-sized supplies, where data and resources rarely support highly subdivided models. In many applied settings, the alternative is not a more complex heterogeneity-resolving model, but a deterministic delineation under the same homogeneous assumption. The workflow therefore provides a pragmatic improvement by quantifying how sensitive the delineation is to uncertainty in the effective parameter values used in that conceptualization. Where data and decision context justify greater detail, heterogeneity can be introduced through zonation or conditional simulation of spatial parameter fields [32, 38], at the cost of additional data requirements, assumptions, and computational effort.

Third, although AEM is computationally efficient, Monte Carlo coupling increases runtime as the number of realizations grows, and post-processing can add additional

workload. In the present study runtimes were manageable, but larger domains or more complex conceptual models may require larger ensembles to obtain stable percentile-based delineations.

The workflow is intended as a first screening-level assessment for sites with limited, but not absent, data and resources, where uncertainty should be considered but a more advanced analysis is not feasible. In this sense, it is meant as a practical first step rather than a substitute for more detailed investigation. It can help show where the site stands with the available information and whether the resulting uncertainty, including the breadth of the WHPA and the range of potentially affected land uses or stakeholders, is acceptable for planning purposes. If not, the results can also indicate that additional data and resources may be needed to support a narrower and more constrained delineation. The approach is particularly aimed at rural or semi-urban settings, where a first transparent indication of possible land-use restrictions may already be useful for groundwater protection planning.

Finally, the percentile-based WHPA envelopes presented here provide a compact summary of how delineation extent changes across the Monte Carlo ensemble. They summarise the ensemble into user-selected percentile envelopes, where lower percentiles yield larger, more precautionary WHPAs. Their width should, however, be interpreted carefully, as it reflects not only the modelling approach but also the hydrogeological setting and the uncertainty in the available data. Broad envelopes may therefore reflect genuine site uncertainty, not only methodological pessimism. At the same time, the presented WHPAs remain conditional on the adopted conceptual model and sampling assumptions. If location-specific capture probabilities are needed, additional post-processing would be required (for example, computing spatial frequencies of inclusion across realizations).

Overall, the workflow prioritizes transparency and usability so that uncertainty-aware WHPA delineation becomes feasible in practice. As highlighted by Höglund et al. [16], uncertainty is often neglected or treated superficially in applied work, and overly complex methods can create barriers to uptake. The open-source implementation provided here is therefore intended as a baseline that can be extended as data availability and decision needs increase.

5.3 Probabilistic wellhead protection areas enhance risk assessments

Improving WHPA delineation is important for safeguarding groundwater sources, particularly for small systems that may be more vulnerable to contamination events because they often rely on groundwater with limited treatment [39]. In these settings, detailed site investigations and fully calibrated numerical models are frequently difficult to justify within available budgets, timeframes, and staffing. The workflow presented here is intended to bridge that gap by enabling uncertainty-aware WHPA delineation within an accessible and reproducible computational setup. It targets practitioners with basic hydrogeological and GIS experience and does not require specialist expertise in numerical modelling or advanced statistics. By integrating pre-processing, modelling, and GIS-ready post-processing in a single Python environment, the approach also reduces the fragmentation that can occur when methods are implemented across multiple software platforms, improving transparency and reproducibility.

Probabilistic delineations can also support risk communication, not only technical risk assessment. Communicating uncertainty in drinking water protection has been identified as a key need, particularly to strengthen collaboration and public awareness around potential contamination risks [40]. In many applied settings, the focus naturally lies on establishing a single defensible delineation, and uncertainty may remain implicit. Fischhoff [41] describes an early stage of risk communication as “all we have to do is get the numbers right”, highlighting that technical results alone do not necessarily translate into shared understanding or action. Presenting percentile-based WHPA envelopes offers a practical way to make uncertainty visible, for example by showing how protection-zone extent changes across plausible parameterizations. This can help decision-makers and stakeholders discuss trade-offs between precaution and the extent of land-use constraints in a more concrete and transparent way.

Finally, a risk-based approach to groundwater protection inherently requires consideration of uncertainty, and regulatory guidance in several contexts has moved toward more comprehensive and risk-informed protection strategies. In Sweden, for example, recent guidance emphasises risk-based work and the need to consider uncertainties in protection planning [14]. Practical probabilistic WHPA tools can support implementation of such frameworks, particularly for small and medium-sized supplies that need methods that are both defensible and feasible to apply.

6 Conclusions

Probabilistic delineation makes WHPAs more defensible because it turns an implicit assumption into an explicit choice: how conservative should a protection boundary be under unavoidable hydrogeological uncertainty. In the Varum case study, percentile-based WHPA envelopes expanded from 3.23 ha (50th percentile) to 102.10 ha (99th percentile), demonstrating how uncertainty can materially change which land uses fall inside a protection zone and, therefore, which restrictions may be considered. Benchmarking against an existing numerical model placed the deterministic pathlines in the central part of the probabilistic ensemble (between the 25th and 50th percentiles), supporting the interpretation that conventional “best-estimate” delineations capture a mid-range outcome rather than a precautionary bound.

For small and medium-sized water supplies, where time, data, and specialist modeling capacity are often limited, this matters in a particularly practical way. The workflow provides an accessible route to uncertainty-aware WHPA delineation and GIS-ready outputs that span central to conservative assumptions, enabling clearer discussions with stakeholders about proportional restrictions and acceptable risk. In this way, probabilistic WHPAs can strengthen risk-based source protection for systems that would otherwise rely on a single deterministic boundary despite substantial uncertainty.

Supplementary Information

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Supplementary Material 1.

Author contributions

Conceptualization, N.G.; Methodology, N.G. and M.Z.; Software, N.G. and M.Z.; Validation, N.G. and M.Z.; Formal Analysis, N.G. and M.Z.; Investigation, N.G. and M.Z.; Data Curation, N.G. and M.Z.; Writing – Original Draft Preparation, N.G.; Writing – Review & Editing, N.G., M.Z. and A.L.; Visualization, N.G.; Funding Acquisition, A.L.

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Data availability

All relevant data are included in the paper or its Supplementary Information.

Declarations

Ethics approval and consent to participate

Not applicable.

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