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Chantal de Fouquet, Mathieu Le Coz, Xavier Freulon, Lea Pannecoucke. Making kriging consistent with flow equations: application of Kriging with Numerical Covariances for estimating a contamination plume. *Hydrogeology Journal*, 2023, 31 (6), pp.1491-1503. 10.1007/s10040-023-02695-6 . hal-04296682

HAL Id: hal-04296682

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Submitted on 20 Nov 2023

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Hydrogeology Journal

Making kriging consistent with flow equations: application of Kriging with Numerical Covariances for estimating a contamination plume --Manuscript Draft--

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| Manuscript Number: | HYJO-D-22-00436R3 | |
| Full Title: | Making kriging consistent with flow equations: application of Kriging with Numerical Covariances for estimating a contamination plume | |
| Article Type: | Paper | |
| Funding Information: | ANDRA | Not applicable |
| | Programme d'investissements d'avenir | Not applicable |
| Abstract: | <p>When the data are few, kriging hydraulic head or concentration with usual variogram models can lead to physically inconsistent results, because the non-stationarity induced by the flow or transport equations is not taken into account properly. Several methods have been proposed to account for these equations in the geostatistical estimation. A recent and general approach consists in incorporating them through specific covariance models. A set of random fields sampling uncertain parameters (e.g. conductivity) is first used as input of a flow simulator. Empirical "numerical" spatial covariances are then calculated between pairs of points and for the variable of interest (e.g. hydraulic head, concentration) on the corresponding set of flow simulator outputs. These non-stationary "numerical" covariances are consistent with the specific spatial variability of hydraulic head or concentrations. They are used in the estimation. In this paper, flow-and-transport simulations are thus combined with kriging to estimate contaminant concentrations in groundwater. A non-stationary Gaussian anamorphosis is introduced for non-linear estimation so that the estimate of the concentration is positive.</p> <p>The method is first validated on synthetic data and then on real data from a two-dimensional cross-section of an aquifer downstream of a trench containing radioactive waste in the Chernobyl area. Kriging with the output of a simplified flow model as external drift and kriging with numerical covariances reproduce the spatial variability of the contaminant plume much better than usual (ordinary) kriging based on observations only. The comparison between the two best estimators is discussed</p> | |
| Corresponding Author: | Chantal de FOUQUET Mines Paris - PSL Fontainebleau, FRANCE | |
| Corresponding Author Secondary Information: | | |
| Corresponding Author's Institution: | Mines Paris - PSL | |
| Corresponding Author's Secondary Institution: | | |
| First Author: | Chantal de FOUQUET | |
| First Author Secondary Information: | | |
| Order of Authors: | Chantal de FOUQUET | |
| | Mathieu Le Coz | |
| | Xavier Freulon | |
| | Léa Pannecoucke | |
| Order of Authors Secondary Information: | | |
| Author Comments: | Fig 4 has been changed | |

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1 [Making kriging consistent with flow equations: application of kriging with numerical](#)
2 [covariances for estimating a contamination plume](#)

3

4 Chantal de Fouquet^{1*}, Mathieu Le Coz², Xavier Freulon¹, Léa Pannecoucke^{1,2}

5 1. Mines Paris, PSL University, Centre for geosciences and geoengineering, 77300

6 Fontainebleau, France

7 2. Institut de Radioprotection et de Sûreté Nucléaire (IRSN), PSE-ENV/SEDRE/LELI, 92260

8 Fontenay-aux-Roses, France

9 * Corresponding author: chantal.de_fouquet@minesparis.psl.eu

10

11 **ABSTRACT**

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32

33 **Keywords:** Groundwater modelling, Geostatistics, Radionuclide migration, Contamination

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35 **NOTE TO COPYEDITOR – PLEASE INSERT THE FOLLOWING AS A FIRST-PAGE FOOTNOTE**

36 Published in the special issue “Geostatistics and hydrogeology”

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39 **1. Introduction**

40 Estimating the hydraulic head or concentrations of components in groundwater is necessary for
41 drawing a map, locating "at best" new measurements by minimalizing redundancy (Júnez-Ferreira et
42 al., 2013), or solving the inverse problem (Gomez-Hernandez et al., 1997; Angulo et al., 1998; de
43 Marsily et al., 2000). However the head or concentration data are generally few and the kriging
44 estimate of these variables with a usual variogram model is not necessarily consistent with the flow
45 physics. Various methods have been proposed to constrain estimates by flow physics, a synthesis and
46 non-exhaustive review of which is presented here.

47 As the head decreases in the flow direction, it is better to carry out the kriging using a non-stationary
48 model (Kumar, 2007). An anisotropic variogram allows one to particularize the direction of flow at the
49 macroscopic scale. Taking covariates into account allows for improvement of the modelling. Thus,
50 Desbarats et al. (2002) introduce the topography as an external drift of the head, choosing the
51 appropriate support of regularization of the digital elevation model. Varouchakis et al. (2012) make a
52 non-linear estimation of the head (using a Gaussian anamorphosis or a modified Box-Cox
53 transformation), with the necessary correction for the back transformation of the estimated values.
54 On a real case, the cross-validation results are improved compared to the usual kriging.

55 Curvilinear coordinate transformation allows for bringing back the “natural coordinates” of flow, i.e.
56 hydraulic head and stream functions (Roth, 1995; Rivest et al., 2012). In order to explicitly introduce
57 flow physics, Brochu et al. (2003) use the formalism of dual kriging to impose to the estimate the form
58 of the analytical solution of a linear or radial flow calculated for a homogeneous medium. In Rivest et
59 al. (2008) the covariate used as external drift is a « smooth » output of a finite element flow model
60 calculated on an uniform transmissivity field, for which boundary conditions must therefore be
61 specified. Tests on synthetic cases show that the accuracy of the estimate and its realism are improved.
62 The method was applied to the real case of a dam.

63 On a synthetic case in steady state, Yang et al. (2018, 2019) reconstruct a field of concentrations by
64 «physics-informed kriging» or «physics-informed cokriging». The method is based on a regression
65 between observations which are considered as “high fidelity” data, and the average of outputs of flow
66 and transport simulations which are considered as “low fidelity” data. The difference between kriging
67 and cokriging lies in the covariance of the discrepancy between low fidelity data and observations. To
68 improve the modelling, Yang et al. (2018, 2019) suggest a non-stationary model for this discrepancy.

69 In another approach, covariance models are constructed so as to be approximately or accurately
70 consistent with flow equations. In the case of steady-state linear macroscopic flow and in the absence
71 of recharge, the linearization of the differential equation linking perturbations of head and
72 transmissivity provides an approximated solution. Hoeksema and Kitanidis (1984) supposed the head
73 to be stationary. Dong (1989, 1990) gave a general solution within the framework of the intrinsic

74 random function of order-k (IRF-k) theory and applied it to the inverse problem, by cokriging the
75 transmissivity from transmissivity and head data. Hernandez et al. (2003) introduced a source term in
76 the equations for performing geostatistical inversion based on the pilot points method (de Marsily,
77 1978; de Marsily et al., 1984). Zhang and Neuman (1996) generalized the analytical form of the simple
78 and cross-covariance to velocity by crossing two flows with different main directions, for comparing
79 longitudinal and transverse dispersion.

80 However the hypothesis of a uniform head gradient is often too strict. Roth et al. (1998) construct a
81 variogram $\gamma(x, x')$ consistent with a steady state flow model with fixed aquifer geometry and
82 boundary conditions. A set of geostatistical non conditional simulations of the conductivity are used
83 as input of a flow simulation. The variogram $\gamma(x, x')$ is calculated, up to the $\frac{1}{2}$ factor, as the mean
84 square deviation of the head at pairs of points x and x' , computed on a set of flow simulation outputs.
85 The numerical version of simple and cross-variograms (or covariances) between head and
86 transmissivity is then used for cokriging these two variables. These experimental non-stationary
87 variograms are used by Schwelle and Cirpka (2010) to estimate the head and the concentration by
88 conditional expectation, calculated by the median (rather than the mean) on a set of simulations
89 constrained by data from different variables. However, the conditional simulations of the
90 transmissivity (or permeability) they use are obtained by an iterative inverse approach.

91 Pannecoucke et al. (2020) generalize the approach to the vadose zone. Non conditional simulations of
92 saturated hydraulic conductivity are used as input to flow-and-transport simulations of a non reactive
93 contaminant. Boundary conditions can vary between the flow simulations, if these conditions are not
94 precisely known. Applications to a wide variety of problems are presented in Pannecoucke (2020) in
95 two dimensions (2D) or 3D, for spatial or spatio-temporal estimation: delimitation of a contaminated
96 zone at fixed contamination threshold and identification of the associated “uncertainty zone”, back-
97 tracing of the unknown location of a contaminant source, comparison of the estimation with the
98 results of a (real) 3D tracing experiment, etc.

99 This paper presents original results of kriging with numerical covariance, following the approach of
100 Pannecoucke (2020), in order to take into account the heterogeneity of a contamination plume.
101 However an anamorphosis (variable transformation) step is introduced, so that the contamination
102 estimates are positive. This non-stationary anamorphosis is calculated on the set of the outputs of the
103 flow-and-transport simulations. The 2D application cases refer to the highly non-stationary context of
104 a contamination plume from a radioactive waste deposit located near the Chernobyl power station in
105 Ukraine. A synthetic case is first examined and the estimation using real-world data is then discussed
106 for comparing three estimation methods: usual kriging, external drift kriging with a simplified flow
107 simulation as covariate, and kriging with numerical covariance.

108 **2. Methods**

109 **2.1. “Numerical” covariance**

110 In classical kriging approaches, the covariance is inferred from observations of the variable to be
111 estimated. However kriging is more general and can be performed based on non-stationary
112 covariances of type $C(x, x')$. Especially, these covariances can be computed between each pair of grid
113 nodes of the domain from a set of N realizations of the variable (Pannecoucke et al., 2020), such as:

$$114 \quad C(x, x') = \frac{1}{N} \sum_{n=1}^N [Z_n(x) - \overline{Z(x)}][Z_n(x') - \overline{Z(x')}] \quad (1)$$

115 where $C(x, x')$ is the “numerical covariance” between grid nodes x and x' and $Z_n(x)$ (respectively
 116 $Z_n(x')$) is the value of the variable Z at grid node x (respectively x') for the n -th realization. For each
 117 grid node x , the “numerical” covariance at all 2D grid nodes x' draws a 2D map. Fig. 1 shows the maps
 118 of numerical covariances related to two different points x , for a set of simulated concentration plumes
 119 (see further section 3.2.). It can be shown that the numerical covariance $C(x, x')$ (or the numerical
 120 variogram $\gamma(x, x')$) has the required mathematical properties of a (discrete) covariance or variogram
 121 function (de Fouquet, 2019; Pannecoucke, 2020).

122 For the application (Section 3) the realizations of the variable of interest are generated by flow-and-
 123 transport simulations of a contaminant plume. First, a set of geostatistical simulations of the hydraulic
 124 conductivity is constructed and simulations of the source term of the contamination are taken from a
 125 previous work (Nguyen, 2017). The flow-and-transport simulations are based on the synthesis of
 126 several studies (Le Coz et al., 2023). Nevertheless, it should be noted that the influence of the range of
 127 the hydrogeological parameters was reduced compared with the variability between realizations and
 128 with the boundary conditions (Pannecoucke et al., 2019; Pannecoucke, 2020).

129 The kriging with numerical covariance can be seen as a generalization of kriging in natural flow
 130 coordinates. Indeed, a stationary covariance K applied after a space transformation f can be written
 131 as $K(f(x) - f(x'))$ and therefore is of the form $C(x, x')$ when the function f is not linear. Conversely,
 132 in the case of a complex phenomenon, such as the development and movement of a plume, it is not
 133 necessarily the case that a space transformation f and a stationary covariance K exist such that the
 134 non-stationary covariance $C(x, x')$ is of the form $K(f(x) - f(x'))$. It is thus pragmatic to calculate the
 135 empirical non-stationary covariance (the “numerical covariance”) on a set of outputs of the numerical
 136 flow-and-transport simulations.

137 **2.2. Non-stationary Gaussian transformation**

138 In practice, kriging with a numerical covariance does not ensure that the estimated concentration is
 139 positive. The non-linear estimation in the well-known anamorphosed Gaussian model (Chilès and
 140 Delfiner, 2012) allows avoiding negative estimates for positive quantities.

141 Due to the non-stationarity of the local distributions of the simulated contaminant concentrations
 142 (especially, inside vs. outside the contaminant plume), a Gaussian transformation of these distributions
 143 is performed at each grid node. The non-stationary anamorphosis Φ_x is calculated from the N outputs
 144 of the flow-and-transport simulation at the grid node x . Thus:

$$145 \quad Z_n(x) = \Phi_x[Y_n(x)] \quad (2)$$

$$146 \quad \text{and conversely } Y_n(x) = \Phi_x^{-1}[Z_n(x)]$$

147 where $Y_n(x)$ is the Gaussian transform of the contaminant concentration $Z_n(x)$ of the n -th flow-and-
 148 transport simulation at grid node x . Here the anamorphosis is calculated using its Hermite polynomial
 149 expansion (with 30 polynomials; Chilès and Delfiner, 2012).

150 The numerical covariance is then calculated on the set of the N fields of Gaussian transformed
 151 variables.

152 The Gaussian data used for the estimation are deduced from the measurements (or from the reference
153 data in the synthetic case) using the inverse of the anamorphosis (ϕ_x^{-1}). The kriging estimate and the
154 kriging variance are calculated in the Gaussian world.

155 Finally the conditional expectation of the concentration, its quantiles or any related functions, are
156 calculated through the known relationship with the spatial distribution of a Gaussian random function;
157 for example (Matheron, 1976; Chilès and Delfiner, 2012):

$$158 \quad E(Z(x)|Z(x_i), i = 1, \dots, n) = \int \phi_x(Y^*(x) + \sigma(x)u) g(u) du \quad (3)$$

159 where $E(Z(x)|Z(x_i), i = 1, \dots, n)$ is the conditional expectation of the concentration; $Y^*(x)$ is the
160 kriging with known mean (equal to 0), $\sigma(x)$ the standard deviation of the kriging error, g the density
161 of the reduced normal distribution and u is the variable to be integrated. This expression can be
162 calculated using the formula of the Hermite-polynomial expansion of the Gaussian anamorphosis
163 (Chilès and Delfiner, 2012). A known correction is applied on the standard deviation if the kriging with
164 unknown mean (ordinary kriging) is used (Emery, 2006). Equation (3) ensures that the estimated
165 concentration is positive, because the concentrations outputs of the flow-and-transport simulations
166 used for calculating the anamorphosis are positive.

167 **2.3. Estimation workflow with numerical covariances**

168 In summary, the method involves the following steps:

- 169 • simulating a set of unconditional hydraulic conductivity fields (geostatistical unconditional
170 simulations by any classical method, e.g. the turning bands as used here; Chilès and Delfiner, 2012);
- 171 • simulating initial source term of the contamination (geostatistical conditional simulations in the
172 following example)
- 173 • simulating flow-and-transport on each hydraulic conductivity field to obtain a set of concentration
174 fields;
- 175 • calculating the non-stationary anamorphosis of the concentrations at each grid node Φ_x from the
176 set of simulated concentration fields;
- 177 • calculating the Gaussian variable for each simulated concentration field using Φ_x^{-1} ;
- 178 • calculating the numerical covariances from the set of Gaussian variables;
- 179 • calculating Gaussian data as the Gaussian transform of concentrations data using Φ_x^{-1} at data
180 points;
- 181 • kriging of Gaussian variable from Gaussian data and computing associated kriging variance, using
182 the numerical covariances on Gaussian transforms;

- 183 • returning to the estimated concentration (or any function of the concentration, e.g. conditional
184 quantiles or conditional distribution) thanks to Eq. (3)

185 3. Case study

186 3.1. The trench T22 in Chernobyl

187 The Chernobyl accident of April 1986 released large amounts of radionuclides into the surrounding
188 environment. In 1986 and 1987, emergency clean-up was carried out in the irradiated Red Forest, in
189 the vicinity of the Chernobyl nuclear power plant. About $500 \times 10^3 \text{ m}^3$ of contaminated topsoil,
190 vegetation and other radioactive materials were buried in situ in hundreds of trenches dug within the
191 permeable sandy superficial formation, directly above the water table and without engineered
192 moisture-proof barriers (Kashparov et al., 2012).

193 In 1998, an experimental research facility was built around the trench T22 in order to investigate
194 radionuclide migration processes. Then, for about 20 years, the trench T22 has been monitored
195 extensively, allowing an advanced characterization of the site geology, the water flow regime in the
196 unsaturated and saturated zones, the radionuclide distribution, and the speciation within and outside
197 the trench (e.g., Bugai et al., 2012; Kashparov et al., 2012). Moreover, acquired data and knowledge
198 were integrated into numerical models that simulate the migration of radionuclides, especially ^{90}Sr
199 (Strontium-90), from the trench to the underlying aquifer (Bugai et al., 2012; Nguyen, 2017). Le Coz et
200 al. (2023) present a detailed synthesis of previous works used for the flow-and-transport modeling
201 near the trench.

202 3.2. Flow-and-transport simulations

203 Between 2000 and 2015, groundwater was collected for ^{90}Sr activity measurements generally once or
204 twice a year at four sampling depths (layers L1 to L4, from top to bottom) in six wells (AP1 to AP6, from
205 upstream to downstream) along a cross-section A-B, approximatively perpendicular to the trench T22
206 and assumed to be parallel to the groundwater flow lines (Fig. 2 a). A groundwater flow-and-transport
207 model was used for simulating in 2D, i.e. along the vertical cross-section A-B (Fig. 2 b), the development
208 of the ^{90}Sr plume highlighted by this monitoring (Le Coz et al., 2023). Model parameters were constant
209 for each geological unit: eolian deposits, alluvial deposits with floodplain or channel facies (Le Coz et
210 al., 2023). These parameters, as well as the boundary conditions, were set such that the simulated
211 time series of ^{90}Sr activity were consistent with most of the measurements. This simulation with
212 especially uniform hydraulic conductivity by geological unit is called the *calibrated simulation*
213 hereafter.

214 For this study, 400 new flow-and-transport simulations are run by considering the uncertainties on the
215 model parameters (e.g., the parameter that governs radionuclide retention on aquifer material) and
216 boundary conditions (e.g., the percolation rate through the trench T22). In addition, for each run,

- 217 • the spatial variability of hydraulic conductivity is simulated through a random field for which
218 the properties are determined based on textural analysis of aquifer material samples (eolian
219 and alluvial sand). T
- 220 • the initial distribution of ^{90}Sr activity within the trench T22 is a geostatistical conditional
221 simulation (Fig. 2 b) constructed from both *in situ* emission profiles and laboratory analysis of
222 waste samples (Nguyen, 2017).

223 **3.3. Spatial estimation**

224 A set of 357 simulated fields (some simulations did not converge) of the ^{90}Sr activity in the saturated
225 zone along the cross-section A-B is extracted from the flow-and-transport simulations on 1st October
226 2006 (01/10/2006). On this date, the ^{90}Sr activity was measured in groundwater collected at all
227 sampling depths in wells AP1 to AP6 (Fig. 2 b). On the *calibrated* simulation, the ^{90}Sr plume extends up
228 to 40 m from the trench with a downward component (Fig 3a). The geometry of the plume in the
229 simulation set is similar, although its extent varies significantly (e.g., Fig 3b). The distribution of the ^{90}Sr
230 activities computed from the simulation set at the sampling wells shows significant ranges, especially
231 in the core of the plume (highest values) (Fig. 4), yet these ranges generally include the activity of the
232 *calibrated simulation* and of the measurements.

233 Three estimation methods of the ^{90}Sr activity are compared in a cross-validation approach: (i) ordinary
234 kriging (OK); (ii) kriging with an external drift (KED), the drift being the ^{90}Sr activity field extracted from
235 the *calibrated simulation* (Fig. 3a); and (iii) kriging with numerical covariances (KNC) using a non-
236 stationary Gaussian transformation, with covariances computed on the Gaussian transforms of the
237 simulated fields of ^{90}Sr activity (simulations 2 to 357).

238 First, the simulated field 1 (Fig. 3b) is used as a synthetic case in order to compare the results with a
239 known “reality” (this field is not considered for the covariance computation). Estimations are
240 conditioned (i) at the wells AP1 to AP6 and then (ii) only at the most downstream well (AP6), the ^{90}Sr
241 activity at the wells AP1 to AP5 being used for the assessment.

242 Then the actual measurements are considered. As for the synthetic case (ii) the estimations are
243 performed only with the data belonging to the most downstream well (AP6), the ^{90}Sr activity at the
244 wells AP1 to AP5 being used for the assessment.

245 **4. Results**

246 **4.1. Synthetic case**

247 The ^{90}Sr activities extracted from the simulated field 1 (i.e. the synthetic data) at the sampling locations
248 are relatively high with respect to the activities extracted from the other simulations, included the

249 *calibrated* one (Fig. 4). At the wells, the relationship between activity "data" and covariate (*calibrated*
250 simulation) is approximately linear (Fig. 4).

251 Pragmatically, OK and KED kriging are done using an isotropic linear variogram, for avoiding the
252 variogram fitting phase under unfavorable conditions (few data and high variability). When all data at
253 the wells AP1 to AP6 are used in the estimation, the OK estimation (Fig 5a) is consistent with the
254 simulated field 1 (Fig. 3b) only close to these wells, whereas the KED and the KNC estimations (Fig. 5 b
255 and c) reproduce the geometry (extent and downward component) of the ⁹⁰Sr plume on the whole
256 modeling domain. In addition, OK and KED result in negative ⁹⁰Sr activity estimated values in the
257 bottom part of the domain, below the ⁹⁰Sr plume. KED and KNC are similar according to the root mean
258 square error (RMSE) criterion (Tab. 1).

259 When only synthetic data at the well AP6 are used, the geometry of the ⁹⁰Sr plume is still well
260 reproduced by KED and KNC but not at all by the OK (Fig. 6). KED results in negative concentrations
261 outside the ⁹⁰Sr plume. The RMSE criterion calculated on all nodes (Tab. 1), or on the five validation
262 wells only, favors the KNC, and it is nearly the same for the other statistical criteria (Fig. 7 and Tab 2).

263 A scatter diagram between the estimate and "reality" (Fig. 8) confirms the good accuracy of KED and
264 KNC.

265 A test with the average of the 356 others simulations (instead of the *calibrated* simulation) as external
266 drift leads to very similar results, only slightly less precise.

267 **4.2. Actual measurements**

268 The actual measured ⁹⁰Sr activities at some sampling locations differ significantly from the activities
269 extracted from the *calibrated simulation*, but are generally (except in one location) included in the
270 range of activities extracted from the 357 additional simulations (Fig. 4). The relationship between the
271 activity at the wells and the covariate is no longer linear.

272 As for the synthetic case, when the estimations are conditioned by the actual measurements at the
273 well AP6, OK does not reproduce the lateral variability of the ⁹⁰Sr activity with depth (Fig. 9a). KED
274 maintains the geometry of the ⁹⁰Sr plume of the *calibrated simulation*, although the simulated activity
275 is about a half order of magnitude lower (Fig. 9b). The geometry of the ⁹⁰Sr plume estimated by KNC
276 differs significantly: its extent is reduced but the ⁹⁰Sr activity in its core is higher (Fig. 9c). At the five
277 validation wells, all estimates are positive. The relative performances of KED and KNC are here more
278 difficult to decide, because the "best" method varies according to the criterion (Fig. 10 and Tab. 3): the
279 mean error is smaller for KNC, the median error and the RMSE are similar for the two methods,
280 whereas the mean absolute error favors the KED. The scattered points between the estimates and
281 observations are in this case further away from the first bisector (Fig. 11). This confirms the greater
282 inaccuracy than for the synthetic case.

283 **5. Discussion and conclusion**

284 The main processes that govern the development of a contaminant plume in groundwater can be
285 simulated using a flow-and-transport model. However, due to uncertainties in input data or
286 misrepresentation of some sub-processes, model output cannot be considered as an accurate

287 representation of the spatial distribution of the contaminant in groundwater at a given date. Usual
288 kriging, e.g., ordinary kriging (OK), offers an alternative, but a high density of observations is necessary
289 for providing realistic estimations. When observations are scarce, geostatistical approaches that take
290 account of physically-based information, e.g., kriging with external drift (KED) or kriging with numerical
291 covariance (KNC), are more relevant.

292 In KED, physically-based information consists of one or several drifts, which governs the geometry of
293 the estimated contaminant plume. Following the literature, the output of a simplified flow model,
294 namely with constant conductivity, is chosen here as external drift. KED requires, therefore, only one
295 flow-and-transport simulation. In the case of actual observations, this drift is not necessarily consistent
296 with those data; then KED could modify the variability of the estimated concentrations (location and
297 level) of the plume.

298 With KNC, a set of several hundred flow-and-transport simulations are used as physically-based
299 information for computing the numerical covariances (and optionally the non-stationary
300 anamorphosis). On synthetic cases, when the observations are consistent with the simulation set (i.e.,
301 when observations are extracted from one reference simulation), the geometry of the contaminant
302 plume of the reference simulation is fairly well reproduced. In the case of actual observations, the
303 geometry of the contaminant plume could significantly differ from that of the simulated plumes. If the
304 numerical covariance does not reflect this discrepancy, then the KNC will lead to inaccurate results.
305 For the actual measurements of the trench T22, the estimated concentrations seem more contrasted
306 with KNC than with KED (Fig. 9), with larger maximum values. In addition, in all cases, concentration
307 fields estimated by KNC associated with a Gaussian anamorphosis are strictly positive.

308 These results corroborate the conclusions of the previous work of Pannecoucke et al. (2020), which
309 focused on a synthetic case that represents the development of a contaminant plume in the
310 unsaturated zone. Indeed, this study, based on a real dataset from the saturated zone, confirms that
311 the non-stationary numerical covariances allow integrating phenomenological knowledge in the
312 kriging estimation. Moreover, it also shows that kriging with numerical covariance could be more
313 accurate than external drift kriging, which does not consider the uncertainties related to this covariate,
314 especially when the geometry of the contaminant plume is complex. The quality of the estimation
315 depends on the ability of the physically-based realizations used for computing the numerical
316 covariances to be consistent with the actual flow-and-transport processes and the corresponding
317 uncertainties.

318 However, the (unique) simplified flow-and-transport simulation used as drift for the KED requires a
319 much lower calculation time than the set of simulations needed for computing the numerical
320 covariances. One reviewer points out that “the workflow needed for the KNC also requires a consistent
321 number of additional steps as compared with the other alternatives.”

322 Rather than a new "better method", kriging with numerical covariance appears to be an alternative to
323 external drift kriging, which enriches the estimation methods useful to the practitioner. This general
324 method can be applied to diverse issues in hydrogeology, in multivariate or spatio-temporal modeling,
325 when estimating or conditioning simulations of hydraulic head or fluxes, backtracking of a plume to
326 locate the source of a pollution (Pannecoucke, 2020), and in hydro-geochemical modelling. The
327 method obviously applies to other contexts (e.g. air quality), and provides a very general class of
328 covariances, e.g. on graphs or other non-Euclidean geometry.

329

330 **Acknowledgments**

331 The authors cordially thank the reviewers and editor whose comments greatly helped to improve the
332 paper. Following the remarks of one reviewer, the “calibrated” simulation was used as external drift,
333 in preference to the average of the set of simulations.

334

335 **Funding Information and Conflicts of Interest**

336 This study benefited from the Kri-Terres project, supported by the French National Radioactive Waste
337 Management Agency (ANDRA) under the French “programme d’investissements d’avenir”.

338 The authors declare there is no conflict of interest in connection with the submitted material

339

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436 effects on advective transport. *Water resources research*, 32(1) 77-83

437

438

439 **Figure captions**

440 Figure 1a,b. Examples of numerical covariance maps, for two different points x (red circles).

441 Figure 2. Views of the 3-D model of the ^{90}Sr inventory in 1987 in the trench T22 (computed from the
442 mean inventory estimated by Nguyen, 2017) and locations of the wells monitored for groundwater
443 activity. (a) Horizontal view with cumulative ^{90}Sr activity in depth; (b) vertical cross-section A-B .

444 Figure 3. Activity of ^{90}Sr in the saturated zone downstream of the cross-section A-B of the trench T22
445 simulated with the flow-and-transport model on 01/10/2006: (a) *calibrated* simulation used as
446 external drift; and (b) simulation 1 taken as reference for the synthetic case study

447 Figure 4. ^{90}Sr activity at the sampling locations. Scatter diagram between (a) the synthetic case in
448 abscissa (horizontal axis) and the *calibrated* simulation in ordinate (vertical axis) and (b) the actual
449 measurements (horizontal axis) and the *calibrated* simulation in ordinate, . The grey bar represents
450 the range of the set of 357 simulations. The black line corresponds to the first bisector.

451 Figure 5. Synthetic case (i.e., flow-and-transport simulation 1). Activity of ^{90}Sr in the saturated zone
452 downstream of the cross-section A-B of the trench T22 (Fig. 2) estimated on 01/10/2006 conditioned
453 at wells AP1 to AP6: (a) ordinary kriging (OK); (b) kriging with external drift (KED); and (c) kriging with
454 numerical covariances using a non-stationary Gaussian transformation (KNC). The non-filled areas (in
455 a and b) correspond to negative estimated activities.

456 Figure 6. Synthetic case. Activity of ^{90}Sr in the saturated zone downstream of the cross-section A-B of
457 the trench T22 (Fig. 2) estimated on 01/10/2006 conditioned at well AP6 only: (a) ordinary kriging
458 (OK); (b) kriging with external drift (KED); and (c) kriging with numerical covariances using a non-
459 stationary Gaussian transformation (KNC). The non-filled area (in b) corresponds to negative estimated
460 activities.

461 Figure 7. Synthetic case. Profiles of estimated activity by OK, EDK or KNC at wells AP1 to AP5,
462 conditioned by “data” at well AP6 and “reality”. Logarithmic scale.

463 Figure_8. Synthetic case. Scatter diagram between estimate (abscissa) and reference value (ordinate)
464 for the three estimation methods (OK, KED, KNC) at the five validation wells for the estimation from
465 AP6.

466 Figure 9. Activity of ^{90}Sr in the saturated zone downstream of the cross-section A-B of the trench T22
467 (Fig. 2) estimated on 01/10/2006 conditioned with measurements at well AP6: (a) ordinary kriging
468 (OK); (b) kriging with external drift (KED); and (c) kriging with numerical covariances using a non-
469 stationary Gaussian transformation (KNC). The non-filled area (in b) corresponds to negative estimated
470 activities.

471 Figure 10. Profiles of estimated activity by OK, EDK or KNC at wells AP1 to AP5, conditioned by actual
472 measurements at well AP6, and validation measurements. Logarithmic scale.

473 Figure 11. Actual measurements. Scatter diagram between estimate (abscissa) and exact value
474 (ordinate) for the three estimation methods (OK, KED, KNC) at the five validation wells for the
475 estimation from AP6.

476 **Tables**

477 Table 1. RMSE at all 1785 grid nodes, for the two conditioning sets of wells. The very weakly negative
 478 values of KED are retained. The numbers have been rounded

| Well set | OK | KED | KNC |
|---------------------------|------|------|------|
| 6 conditioning wells | 363. | 102. | 106. |
| 1 conditioning well (AP6) | 658. | 135. | 94. |

479

480

481 Table 2. Cross-validation statistics at the five validation wells (AP1 to AP5, 20 values) estimated from
 482 the data of the AP6 well, for the synthetic case. Negative estimates are zeroed for the statistics of the
 483 error, but their number is reported. The error is calculated as *estimate – exact data*.

| Statistic | OK | KED(0) | KNC |
|------------------------------|-------|--------|------|
| Mean error | -127. | -103. | 3. |
| Median error | 306. | 0. | 10. |
| Mean absolute error | 692. | 134. | 87. |
| RMSE | 908. | 227. | 135. |
| Number of negative estimates | 0 | 9 | 0 |

484

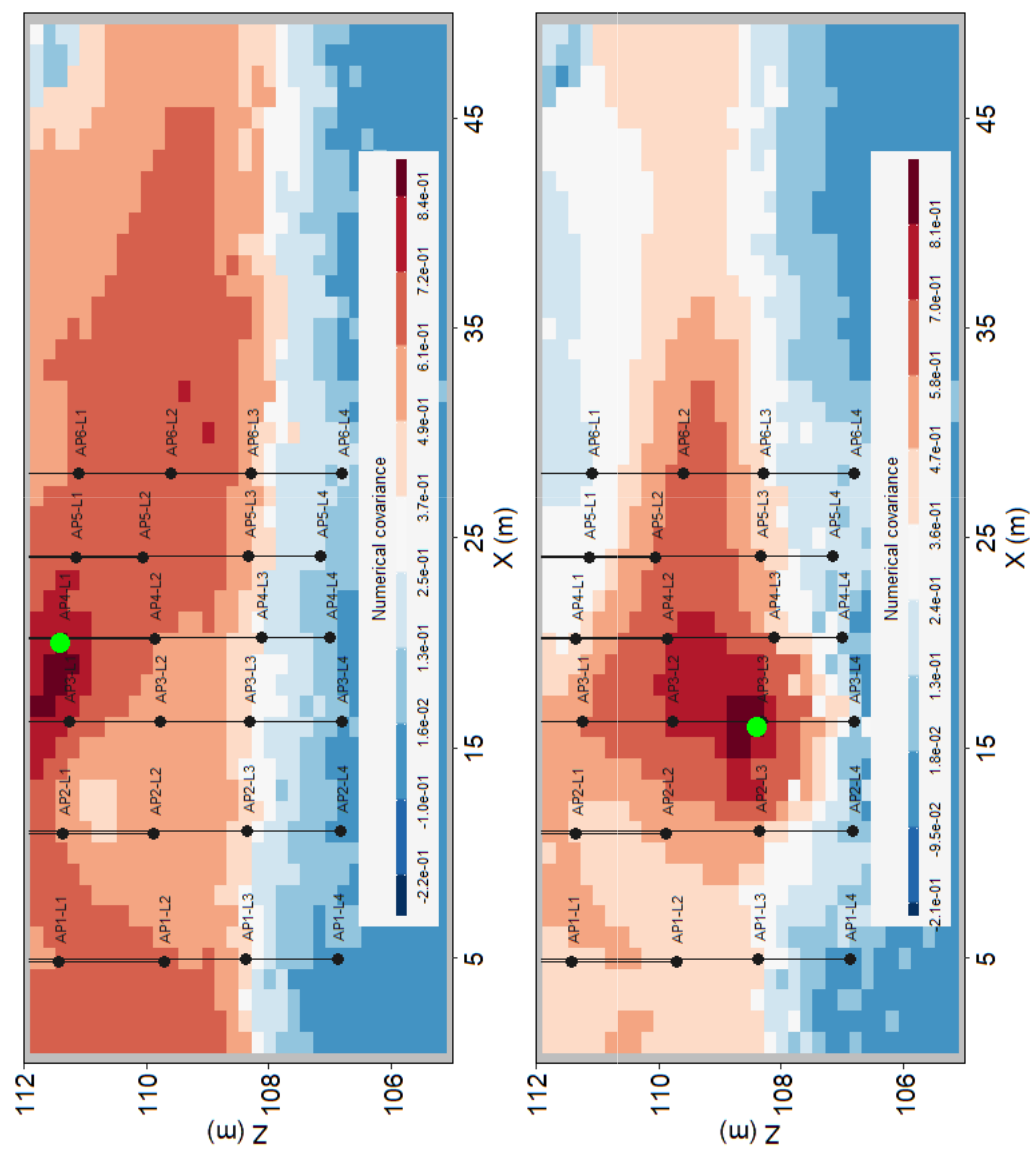
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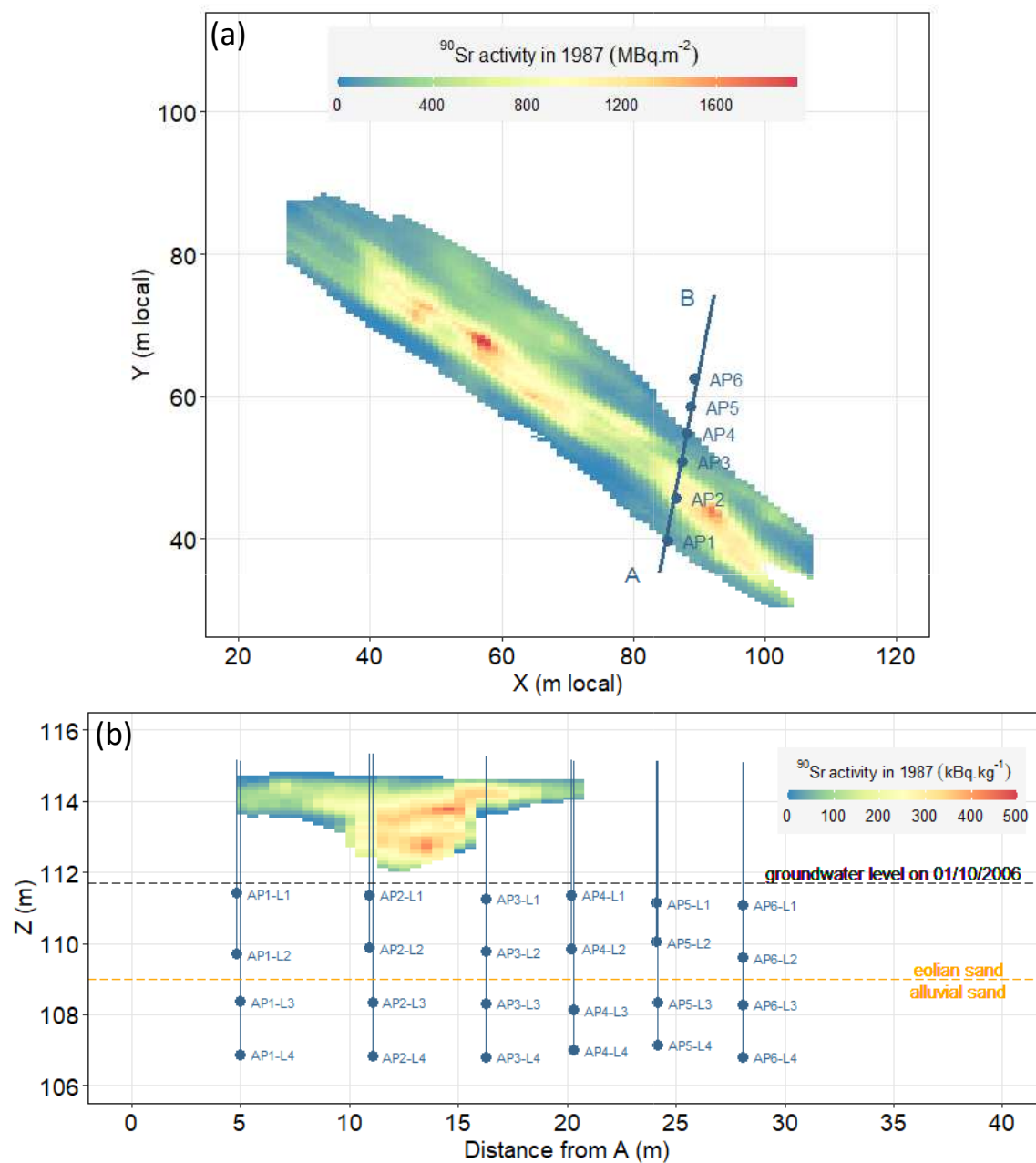
486 Table 3. Cross-validation statistics at the five validation wells (AP1 to AP5, 20 values) estimated from
 487 the data of the AP6 well, for the actual measurements.

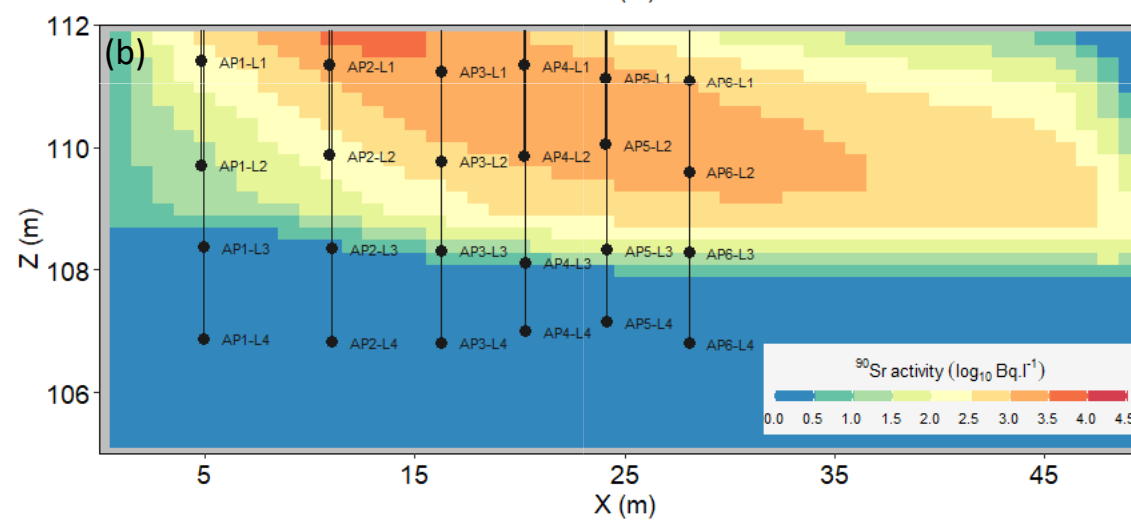
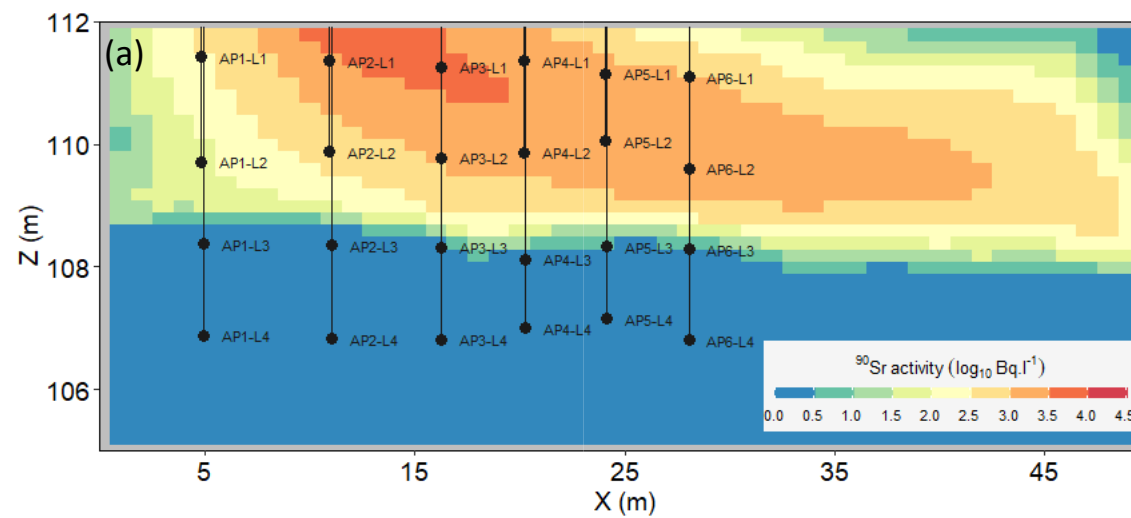
| Statistic | OK | KED | KNC |
|------------------------------|-------|-------|------|
| Mean error | -199. | -195. | -80. |
| Median error | 37. | 0. | -3. |
| Mean absolute error | 312. | 227. | 267. |
| RMSE | 589. | 472. | 477. |
| Number of negative estimates | 0 | 0 | 0 |

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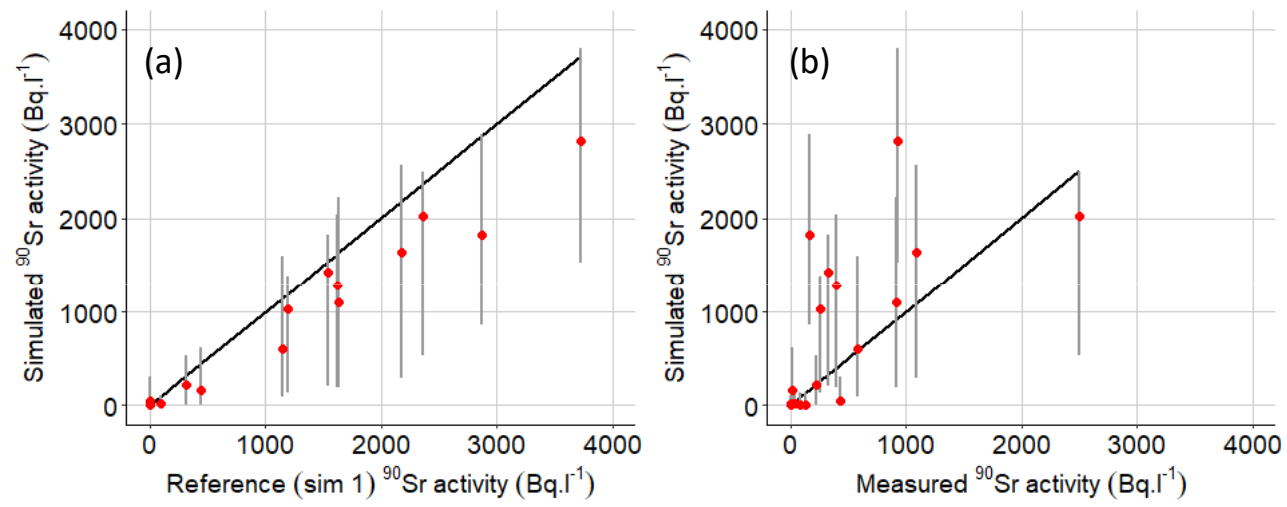


Figure 5

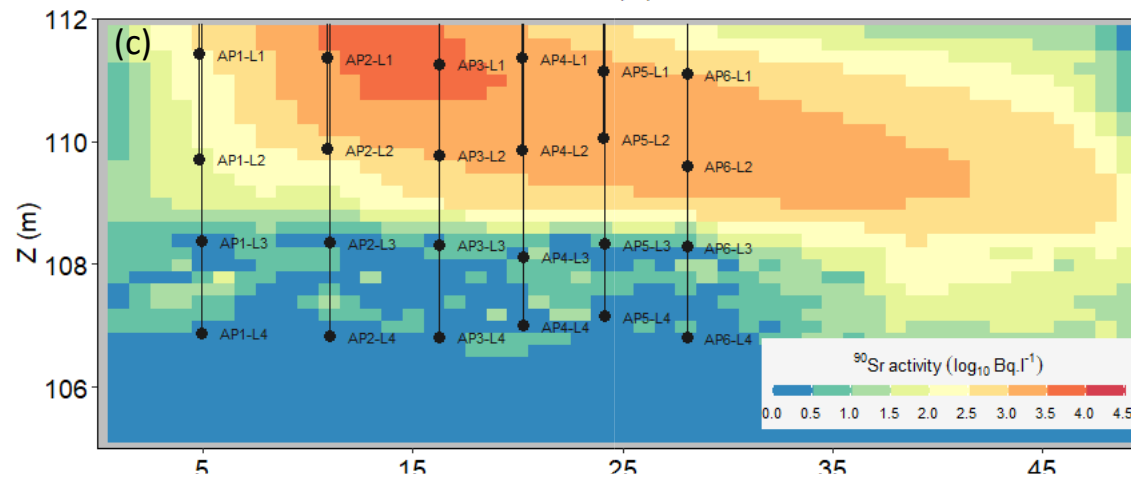
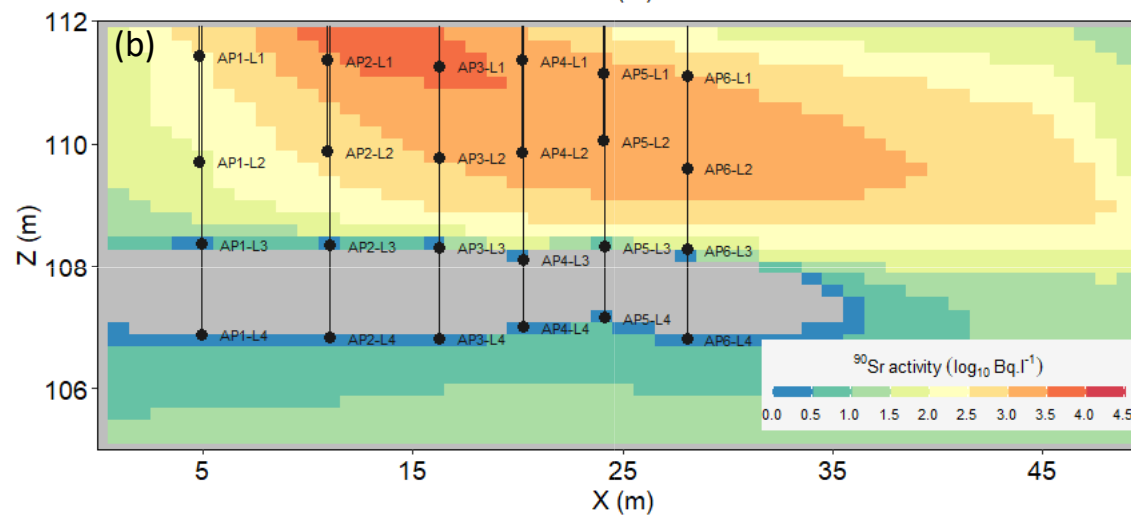
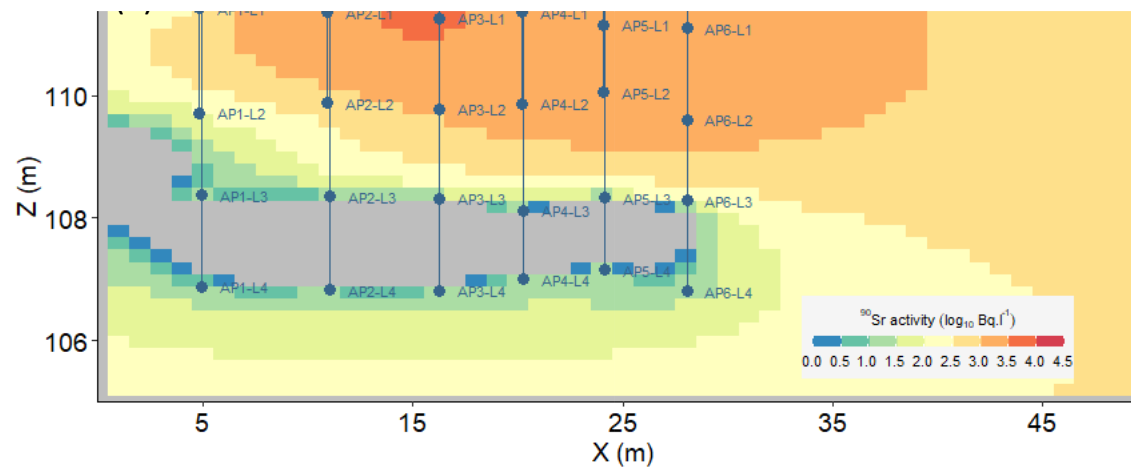
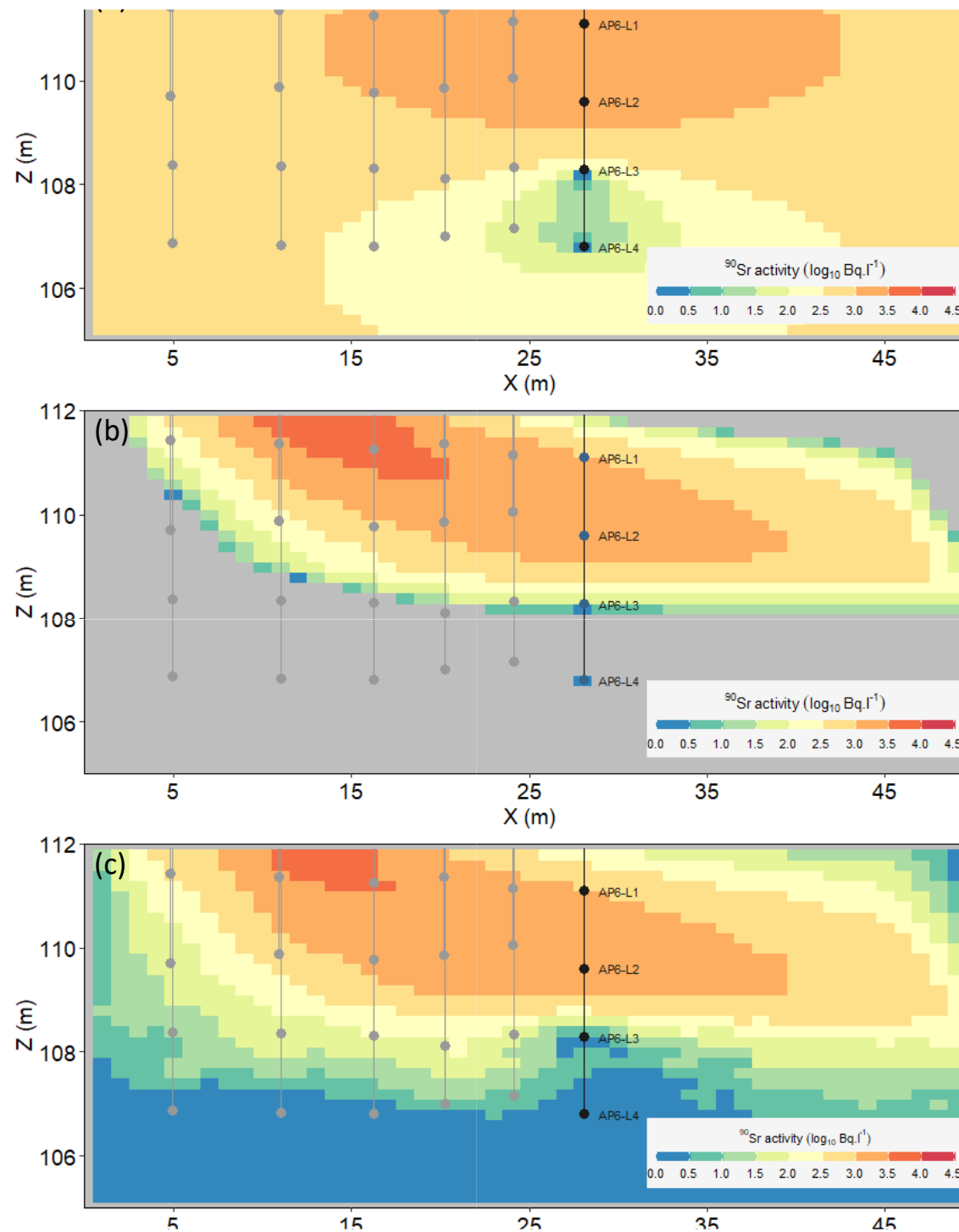
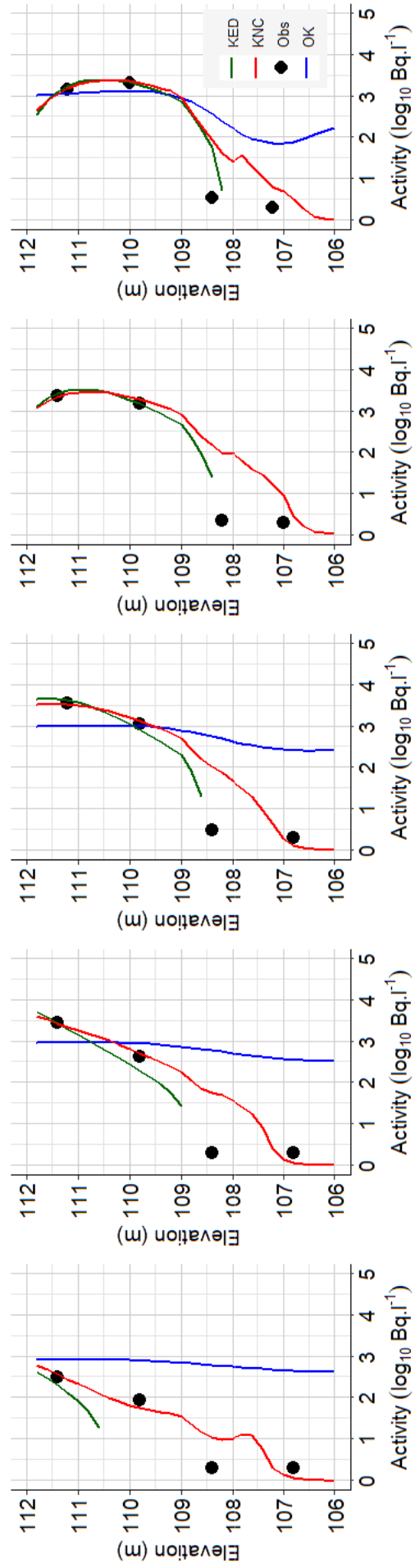


Figure 6





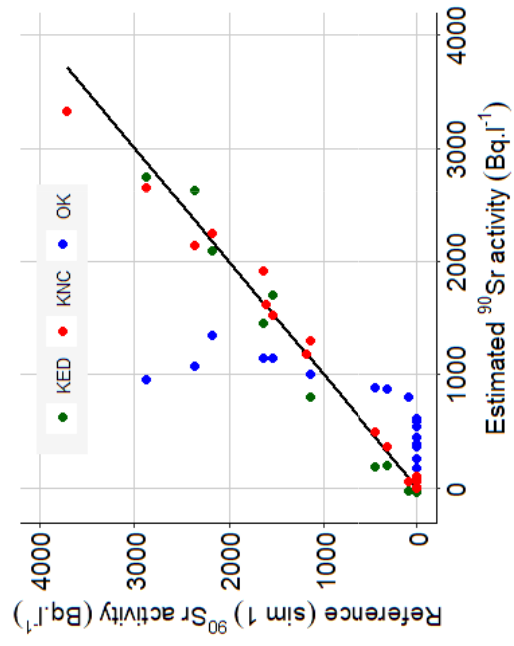
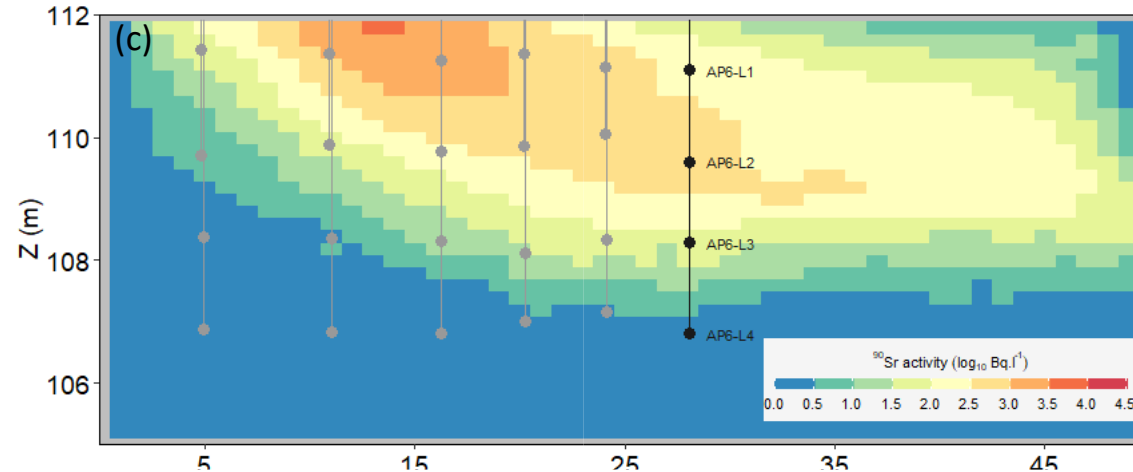
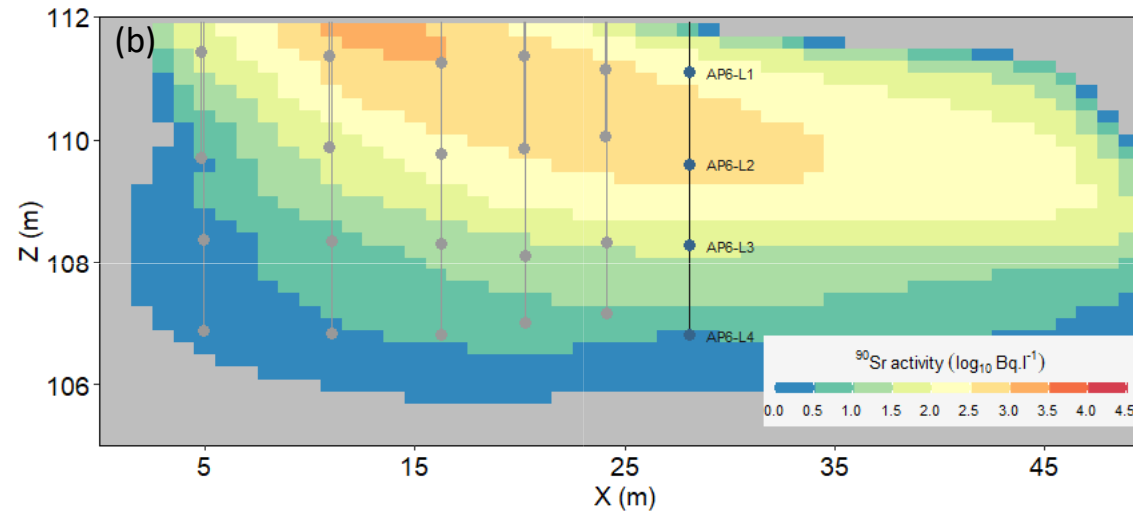
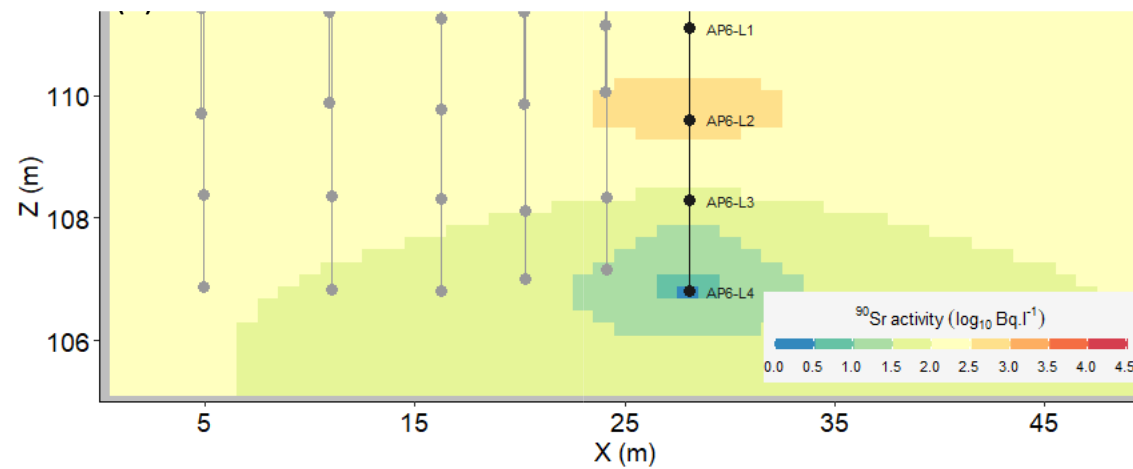
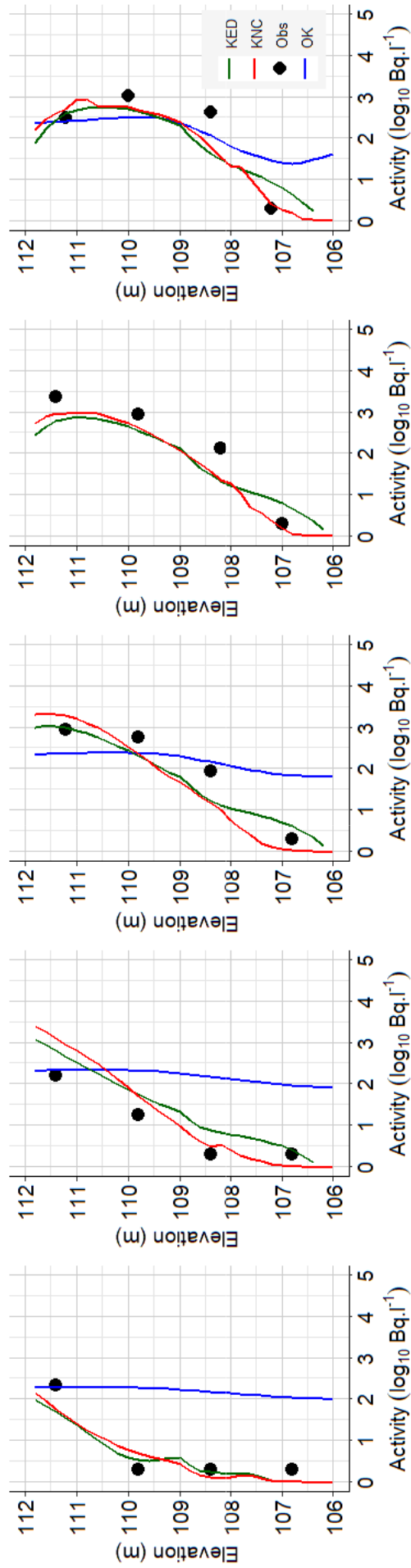
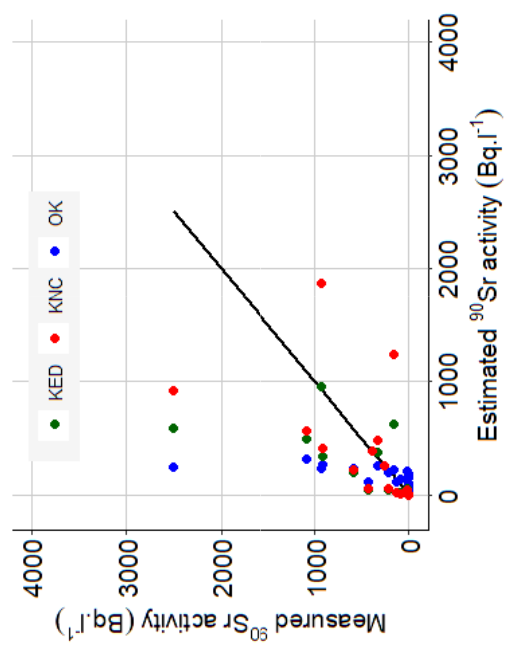


Figure 9







There are no comments