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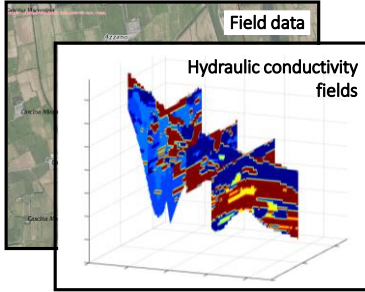
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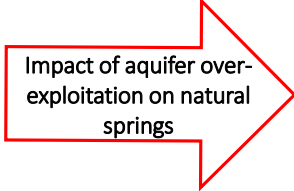
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# Graphical abstract

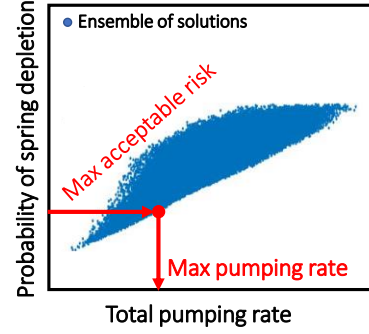
## GROUNDWATER FLOW MODELS



Parameter and conceptual model uncertainty



## PROBABILISTIC RISK ANALYSIS



**Highlights:**

- Probability of spring discharge reduction due to aquifer exploitation is quantified
- Multiple sources of uncertainty are considered using a Fault Tree methodology
- The approach balances conflicting goals under parameter and conceptual uncertainty

1 **Natural springs protection and probabilistic risk assessment under uncertain conditions.**

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- 13 • Probability of spring discharge reduction due to aquifer exploitation is quantified
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## Abstract

The study introduces a comprehensive framework for natural springs' protection and probabilistic risk assessment in the presence of uncertainty associated with the characterization of the groundwater system. The methodology is applied to a regional-scale hydrogeological setting, located in Northern Italy and characterized by the presence of high-quality natural springs forming a unique system whose preservation is of critical importance for the region. Diverse risk pathways are presented to constitute a fault tree model enabling identification of all basic events, each associated with uncertainty and contributing to an undesired system failure. The latter is quantified in terms of hydraulic head falling below a given threshold value for at least one amongst all active springs. The workflow explicitly includes the impact of model parameter uncertainty on the evaluation of the overall probability of system failure due to alternative groundwater extraction strategies. To cope with conceptual model uncertainty, two models based on different reconstructions of the aquifer geological structure are considered. In each conceptual model, hydraulic conductivities related to the geomaterials composing the aquifer are affected by uncertainty. It is found that (a) the type of conceptual model employed to characterize the aquifer structure strongly affects the probability of system failure and (b) uncertainties associated with the ensuing conductivity fields, even as constrained through model calibration, lead to different impacts on the variability of hydraulic head levels at the springs depending on the conceptual model adopted. The results of the study demonstrate that the proposed approach enables one to (i) quantify the risk associated with springs depletion due to alternative strategies of aquifer exploitation; (ii) quantify the way diverse sources of uncertainty (i.e., model and parameter uncertainty) affect the probability of system failure; (iii) determine the optimal exploitation strategy ensuring system functioning; and (iv) identify the most vulnerable springs, where depletion first occurs.

## 1. Introduction

Population growth, urbanization and the pursuit of improved living conditions accelerate the need for water, food and energy. Freshwater is a limited resource (only 0.7% of the global water resource is readily available as freshwater) and its availability is a key driver of population dynamics. Groundwater, which is the main source of available freshwater in many countries worldwide (Filimonau and Barth, 2016), is a strategic resource for drinking water supply and is essential for ecosystem quality, energy and food security. Groundwater is at risk from a variety of causes, including over-abstraction, with about 20% of the world's aquifers being estimated to be suffering from over-exploitation (e.g., Amanambu et al., 2020, Jia et al., 2020, Jia et al., 2019, Castellazzi et al., 2016, Gleeson et al., 2012). Groundwater abstraction close to natural springs, which represent key elements of a hydrological system, requires an appraisal and quantification of possible interference between pumping and head levels at the springs, as well as an assessment of the complexity of environmental, social and economic aspects (e.g., Obolewsky et al., 2016, Epting et al., 2018, Liu et al., 2018, Luo et al., 2020). For these reasons, groundwater exploitation and management should foresee relying on an approach that enables considering the coexistence of multiple (sometimes conflicting) objectives.

It is widely recognized that uncertainty affects all efforts to model hydrogeological systems. Aquifer heterogeneity and incomplete knowledge of key attributes enabling site characterization are some of the reasons why decisions about groundwater exploitation and management needs to be made under uncertainty. Decisions are typically informed by several alternatives which are rendered through models plagued by diverse sources of uncertainties. Therefore, risk analysis, which is by its nature interconnected with the concept of uncertainty, must be an integral part of any decision-making process associated with environmental scenarios (Bolster et al., 2009, Tartakovsky, 2013). A Probabilistic Risk Assessment (PRA) allows identifying all basic events and possible risk pathways contributing to an undesired system failure in order to quantify the probability that such an event takes place (Bedford and

68 Cooke, 2003). This quantitative tool takes advantage of information from multiple entries of various  
69 origins and synthesize these in a descriptive and simplified set of indicators, easily transferable to  
70 decision makers. Several works show that PRA is a valuable tool for evaluating diverse groundwater-  
71 related types of risks, such as, e.g., (a) probability of failure of a given groundwater remediation  
72 strategy (e.g., Tartakovsky, 2007; Bolster et al., 2009, Fernández-Garcia et al., 2012, Siirila-Woodburn  
73 et al., 2015), (b) events associated with construction of underground structures and their feedbacks with  
74 aquifers (Jurado et al., 2011), and (c) maintenance of artificial recharge ponds (Pedretti et al., 2011).  
75 PRA has also been employed to embed the reconstruction of probabilistic well capture zones (Rodak et  
76 al., 2011) and to evaluate human health risk due to toxic chemical cocktails released in groundwater  
77 (Henri et al., 2015).

78 In this broad context, the development of a structured PRA associated with scenarios of spring  
79 discharge reduction (possibly leading to spring depletion) linked to groundwater over-abstraction is still  
80 lacking. Luo et al. (2020) propose a multi-objective simulation/optimization framework to assess an  
81 optimal strategy which balances groundwater extraction and outflow rate at the Baotu spring field, in  
82 Northern China. In this study, the authors do not include the effects of any source of uncertainty, the  
83 latter being ubiquitous in the representation of subsurface flow and transport processes. Additional  
84 studies about springs and their interconnection with groundwater exploitation mainly focus on the  
85 analysis of the relationships among spring flow, precipitation, and groundwater abstraction, with the  
86 main objective of providing an appraisal, within a deterministic framework, of variations of spring flow  
87 due to climate change and human activities (Kang et al., 2011, Zhang et al., 2017, Liu et al 2018).

88 Our key objective is the development of a methodology to quantify the probability of system  
89 failure associated with the reduction of discharge at natural springs due to aquifer over-exploitation in  
90 the presence of multiple sources of uncertainty. This is accomplished by relying on a Fault Tree  
91 approach.

92 The applicability and performance of the proposed approach and ensuing operational workflow  
93 are shown in an exemplary setting comprising a complex, large scale aquifer system located in  
94 Northern Italy. The target aquifer is characterized by the presence of high-quality natural springs which  
95 constitute the main supply to agriculture and are a key environmental driver for various activities,  
96 forming a unique and highly valuable system whose preservation is of critical importance for the  
97 region. As an additional distinctive element, our study provides a solid probabilistic framework for the  
98 assessment of the best compromise one can obtain by balancing two conflicting goals, as given by the  
99 minimization of the probability of system failure (identified through a reduction of spring discharge  
100 below a given threshold) and the maximization of the water volume that can be extracted from the  
101 aquifer, under uncertain conditions.

## 102 **2. Study area and groundwater flow model**

103 The study is focused on a highly heterogeneous regional-scale sedimentary aquifer, located in  
104 Northern Italy (see Fig. 1). The main hydrogeological features of the system that are essential to the  
105 scope of the present work are illustrated in the following and one can refer to Bianchi Janetti et al.  
106 (2019) for additional details, including the exhaustive description of the available data upon which our  
107 analyses are grounded.

108 The considered region is part of the high-medium Alluvial Po Plain in Northern Italy and extends  
109 across a planar surface of about 785 km<sup>2</sup>. It is located between the two major rivers (Adda and Serio) in  
110 the area and hosts activities linked to agricultural (84%) and urban (16%) sectors. The presence of  
111 high-quality water springs constitutes a key feature of the system. These natural springs are major  
112 environmental drivers and constitute the main water supply for agriculture, which is an important  
113 anthropogenic activity in the area.

114 Main features of the system are depicted in Fig. 1b, which includes the overall pattern of the  
115 groundwater surface elevation as well as the location of springs and of pumping wells considered. The



116 aquifer is characterized by an average thickness of about 120 m (stratigraphic data being available up to  
117 a depth of about 300 m in some areas) and comprises a free-surface (with a few locally semi-confined  
118 conditions) and a deep aquifer. Following Bianchi Janetti et al. (2019), a steady-state groundwater flow  
119 pattern, which is taken to represent an average system behavior, is here considered. This choice is  
120 consistent with the analysis of the series of piezometric records available in the area from 2004 to 2015.  
121 As an example, the yearly-averaged (from 2004 to 2015) hydraulic heads at four observation wells used  
122 for model calibration are depicted in Fig. 1c (the exact position of these observation points is included  
123 in Fig. 1b). This figure shows that the interannual variability of hydraulic head is negligible within the  
124 investigated temporal window. This is also consistent with the purpose of our study, which is to  
125 provide a quantitative tool to support decision makers in the context of management of large-scale  
126 groundwater resources. As mentioned in Section 1, this is accomplished by developing a methodology  
127 conducive to evaluating the probability of system failure accounting for diverse conceptualizations of  
128 the hydrogeological domain and the uncertainty of the associated hydraulic parameters governing  
129 groundwater flow patterns. Our analysis provides information about the mean behavior of the system  
130 on a yearly basis that can be used for a high-level management purpose upon which one can then  
131 prioritize requirements for more detailed, local-scale analyses.

132 In addition, one can also note that for the purpose and level of the risk analysis here considered  
133 the steady-state condition can be viewed as a conservative scenario with respect to a transient regime,  
134 as it is associated with the largest drawdown produced by the system of pumping wells.

135 Numerical analyses presented in Section 3 rely on the widely used and tested computational suite  
136 MODFLOW-2005 (Harbaugh, 2005). Boundary conditions correspond to (a) a total flow rate of 9.65  
137 m<sup>3</sup>/s entering the domain from the Northern boundary and (b) a Dirichlet boundary conditions imposed  
138 along the Adda and Serio rivers which is set to 3 m above the river bottom elevation, consistent with  
139 the mean river bank elevation. The aquifer system of extent 23 km (East-West direction) × 48 km

140 (North-South direction)  $\times$  475 m (depth) is discretized through blocks of uniform size of 100 m  $\times$  200  
141 m  $\times$  5 m, according to available information and computational resources, for a total of 5.2 million  
142 voxels. Inactive cells are inserted to reconstruct the topographic surface of the area and the bottom of  
143 the system, resulting in about one million active cells. Recharge terms included in the study comprise  
144 infiltration from precipitation, irrigation and percolation from channels in the non-urban zones, or  
145 aqueduct and sewage system losses in the urban sector. Since exhaustive and up-to-date records  
146 detailing the exact location of the pumping wells are not available, for the illustration of our approach,  
147 and considering the spatial extent of the system, the total water withdrawal within a given municipality  
148 is assigned to a system of wells located at the center of the municipality itself. Springs are simulated as  
149 drains, their outflow-rate being proportional to the difference between hydraulic head at the spring cell  
150 and elevation of ground level. Additional details are reported in Bianchi Janetti et al. (2019). Consistent  
151 with these authors, uncertainty in the conceptual model employed to characterize the subsurface  
152 architecture and the spatial variability of hydraulic conductivities in the domain are considered and two  
153 conceptual models are implemented according to the steps summarized in the following.

154 On the basis of available data (see Bianchi Janetti et al., 2019), a set of  $n_f = 5$  main geomaterials  
155 (facies) which constitute the geological makeup of the system is identified. Each facies, here denoted as  
156  $M_i$  ( $i = 1, \dots, n_f$ ), is listed in Table 1 together with the corresponding volumetric fraction,  $f_i$ , assessed  
157 from data collected from boreholes within the study area.

158 The three-dimensional distribution of facies within the system is obtained according to two  
159 conceptual models, which are taken to exemplify the way uncertainty about our knowledge of the  
160 internal structure of the aquifer system can be embedded in the probabilistic analysis workflow, other  
161 types of conceptual models being compatible with our approach. These are termed as *Composite*  
162 *Medium (CM)* and *Overlapping Continua (OC)* model (see also Bianchi Janetti et al., 2019). According  
163 to the *CM* approach (e.g., Winter et al., 2003; Guadagnini et al., 2004 and references therein) a single

164 geomaterial with conductivity  $K_j^{CM} = k_i$  (index  $i$  identifying the facies attributed to voxel  $j$ ) is assigned  
 165 to each voxel of the numerical model. In essence, this can be seen as corresponding to a zonation of the  
 166 domain where (in principle) there might be uncertainty in the spatial distributions of the geomaterials  
 167 and in the value of their hydraulic parameters. The *OC* model is grounded on the concept that the  
 168 system can be viewed as a collection of media of differing properties coexisting in space. The idea  
 169 underlying this concept is that each voxel  $j$  of the numerical grid represents a finite volume within  
 170 which all geomaterials can coexist, each being associated with a given volumetric fraction,  $I_{i,j}$ .  
 171 Hydraulic conductivity at voxel  $j$  is evaluated as a weighted arithmetic mean of facies conductivities,  
 172 i.e.,  $K_j^{OC} = \sum_{i=1}^{n_f} I_{i,j} k_i$ , (with  $\sum_{i=1}^{n_f} I_{i,j} = 1, \forall j$ ).

173 The *CM* and *OC* conceptual models have also been employed by Bianchi Janetti et al. (2019)  
 174 who rely on a number of global sensitivity analysis (GSA) techniques to assess the influence of  
 175 uncertain model parameters on the distribution of hydraulic heads in the complex domain considered.  
 176 These authors identified the set of hydraulic parameters which are most influential to hydraulic head  
 177 distributions as log-conductivity values associated with (i) clay, gravel, and fractured conglomerate for  
 178 *CM* and (ii) gravel and fractured conglomerate for *OC*. Here, we perform model calibration by taking  
 179 advantage of these results, the parameters to be estimated corresponding to  $N_p = 3$  and  $N_p = 2$  values of  
 180  $Y_i = \log k_i$  ( $i = 1, \dots, N_p$ ) for *OC* and *CM*, respectively. Entries  $Y_i$  of vector  $\mathbf{Y}$  are estimated through a  
 181 Maximum Likelihood (ML) approach (Carrera and Neumann, 1986), yielding a ML estimate  $\boldsymbol{\mu}$  of  $\mathbf{Y}$   
 182 based on hydraulic head measurements (see Appendix A for details) as well as a the posterior  
 183 covariance matrix,  $\boldsymbol{\Sigma}$ , of the corresponding estimation error.

184

### 185 3. Probabilistic Risk Assessment of the natural springs - groundwater system

186 Development and application of the PRA requires introducing the following set of components  
187 (see, e.g., Tartakovsky, 2013):

188 (1) *Model predictions*, here identified as the system response in terms of hydraulic head values ( $h$ ) at  
189 a given spring location. Values of  $h$  are obtained upon relying on the representation of the  
190 groundwater flow system described in Section 2, as implemented according to the two conceptual  
191 models considered.

192 (2) *System Failure (SF)* event, here identified with the depletion of at least one spring within the  
193 domain. Note that *SF* generally depends on economical/social constraints and its quantification  
194 benefits from feedbacks with local stakeholders and decision makers. For the purpose of our  
195 exemplary analysis, and considering that the area examined is characterized by a high social  
196 impact related to industrial and agricultural activities, our PRA is implemented with the constrain  
197 that hydraulic head of all active springs does not fall below a given threshold value, to guarantee  
198 a minimum flow rate at each spring.

199 (3) *Design variables*, here associated with the operational flow rates at a set of selected pumping  
200 wells within the domain.

201 (4) *Sources of uncertainty*, representing our incomplete knowledge about system functioning. Here,  
202 two sources of uncertainty are considered, as given by (i) the conceptual model employed to  
203 represent the system and (ii) its ensuing model parameters. Conceptual model uncertainty is  
204 included by considering two diverse approaches (i.e., the *CM* and *OC* models described above) to  
205 reconstruct the main hydrogeological features of the system. Model parameter uncertainty is  
206 tackled by considering the  $N_p$  log-conductivity values associated with each of these conceptual  
207 models to be characterized by a multivariate Gaussian distribution with mean  $\boldsymbol{\mu}$  and covariance  $\boldsymbol{\Sigma}$ .  
208 Evaluation of the latter is grounded on an inverse modeling framework performed within a ML

209 approach (see Section 2), where the prior error vector and the posterior residual vector ( $\mathbf{Y} - \boldsymbol{\mu}$ )  
210 are assumed to be multivariate Gaussian.

211 Note that the nature of our study is mainly methodological and is then rendered through an  
212 exemplary application scenario. In this context, results from a participatory process with local  
213 authorities and stakeholders to refine elements and values for system failure and/or the possibility to  
214 broaden the portfolio of scenarios of interest, for example including additional conceptual models  
215 and/or adding different types of sources of uncertainty are fully compatible with the presented  
216 framework and it is envisioned to tackle these elements in the context of future investigations.

217

### 218 **3.1 Fault tree analysis**

219 The probability associated with  $SF$ ,  $P[SF]$ , stemming from the combination of the various sources  
220 of uncertainty illustrated above can be evaluated through a Fault Tree Analysis (FTA) (e.g., Bedford  
221 and Cooke, 2003; Tartakovsky, 2007; Fernàndez-Garcia et al., 2012). A Fault Tree is formed by  
222 considering various potential events, whose inter-connections can be represented with Boolean  
223 operators. Once a Fault Tree is constructed, the probability of each event must be evaluated, thus  
224 enabling assessment of the overall probability that  $SF$  takes place. As described above,  $SF$  is here  
225 associated with the occurrence of hydraulic head values dropping below an imposed threshold,  $h_{TR}$ , at  
226 least in one spring (amongst those considered in the analysis), i.e.,

$$227 \quad h_j(\mathbf{Q}, \mathbf{Y}) - h_{TR,j} < 0 \quad j = 1, \dots, N_s \quad (1)$$

228 Here  $\mathbf{Q}$  is a vector containing the flow rate of each pumping well,  $h_j(\mathbf{Q}, \mathbf{Y})$  is hydraulic head  
229 evaluated at spring  $j$  while wells are operating at the pumping flow rate  $\mathbf{Q}$  within the log-conductivity  
230 field reconstructed (according to the  $CM$  or  $OC$  model) upon relying on vector  $\mathbf{Y}$  (containing log-

231 conductivity values of each geomaterial),  $h_{TR,j}$  is the threshold (minimum hydraulic head) value  
 232 associated with the  $j$ -th spring, and  $N_s$  is the number of springs. Values of the entries of  $\mathbf{Q}$  vary within  
 233 the interval  $[\mathbf{Q}^{\min}, \mathbf{Q}^{\max}]$ ,  $\mathbf{Q}^{\min}$  and  $\mathbf{Q}^{\max}$  denoting vectors whose entries correspond to the lower ( $Q_w^{\min}$   
 234 ) and upper ( $Q_w^{\max}$ ) bounds of  $Q_w$  (with  $w = 1, \dots, N_w$ ), where  $N_w$  is the number of pumping wells in the  
 235 system.

236 The outflow-rate of the  $j$ -th spring,  $Q_{s,j}$ , of planar area  $A_j$  is then evaluated as

$$237 \quad Q_{s,j} = \begin{cases} A_j \frac{K_{d,j}}{e_j} (h_j - h_{0,j}) & h_j > h_{0,j} \\ 0 & h_j \leq h_{0,j} \end{cases} \quad (2)$$

238 where  $h_{0,j}$  is elevation of the spring bottom,  $K_{d,j}$  and  $e_j$  being hydraulic conductivity and thickness of  
 239 the draining bed of the spring, respectively. Knowledge of quantities  $K_{d,j}$  and  $e_j$  allows evaluating the  
 240 leakage coefficient  $l_{d,j} = K_{d,j}/e_j$ , which is here considered as constant (and denoted as  $l_d$ ) for each  
 241 spring. The value of  $l_d$  has been estimated following calibration of each conceptual model illustrated in  
 242 Section 2 on the basis of available data about the total discharge from the springs (see Appendix A).  
 243 The threshold value  $h_{TR,j}$  has been evaluated from (2) to ensure a minimum flow rate,  $Q_{s,j}^{\min}$ , as

$$244 \quad h_{TR,j} = h_{0,j} + \frac{Q_{s,j}^{\min}}{A_j l_d} \quad (3)$$

245 Along the lines of what noted above, it is observed that the specific value of  $Q_{s,j}^{\min}$  to be employed in the  
 246 probabilistic risk analysis can vary for each spring, eventually including elements associated with  
 247 economic and social constraints. For simplicity and ease of illustration we consider the same value of  
 248  $Q_{s,j}^{\min}$  for each spring, hereafter denoted as  $Q_s^{\min}$ , and also choose to employ the same values for the

249 lower and upper bounds of the flow rate extracted at each of the wells considered in the analysis,  
250 hereafter denoted  $Q^{\min}$  and  $Q^{\max}$ .

251 The construction of the Fault Tree is organized upon partitioning the  $N_p$ -dimensional parameter  
252 space  $\mathbf{Y}$  (geomaterial log-conductivities) according to the three following regions: (i) Region A ( $Y_A$ ),  
253 which comprises the subset of combinations of log-conductivity values for which the constraint (1) is  
254 never satisfied; in other words, this region is formed by the collection of the combinations of log-  
255 conductivity values for which depletion of at least one spring is observed even under conditions  
256 corresponding to the minimum pumping rate ( $Q^{\min}$ ) being set at all pumping wells (i.e.,  $SF$  is always  
257 detected); (ii) Region C ( $Y_C$ ) comprises the subset of log-conductivity values for which constraint (1) is  
258 satisfied upon setting the maximum pumping rate ( $Q^{\max}$ ) at all pumping wells, i.e.,  $SF$  is never  
259 detected; finally (iii) Region B ( $Y_B$ ) includes all combinations of values of geomaterial log-  
260 conductivities which do not belong to either Region A or C, i.e., in this case the occurrence of  $SF$   
261 depends on the values of pumping rate assigned to each well.

262 The chain of events leading to  $SF$  is graphically depicted through the Fault Tree included in Fig.  
263 2. The Boolean operators AND and OR applied to two given events  $X$  and  $Z$  are expressed according to  
264 the following notation:  $X$  AND  $Z \equiv X \cdot Z$  and  $X$  OR  $Z \equiv X + Z$ . Therefore, the Boolean expression  
265 corresponding to the Fault Tree in Fig. 2 is

$$266 \quad SF = M_1 + M_2 = Y_A + Y_B \cdot (h_{TR,j} > h_j) \quad (4)$$

267 Equation (4) allows identifying the failure modes ( $M_1$  and  $M_2$ ) of our system (also termed as  
268 *minimal cut sets of the system*) and correspond to the smallest collections of events leading to  $SF$ :

- 269 •  $M_1$ : {‘Values of geomaterial log-conductivities belong to Region A’}

- 270 •  $M_2$ : {‘Values of geomaterial log-conductivities belong to Region B’ AND ‘Hydraulic head  
271 rendered by the model is lower than the threshold for at least one spring’}.

272 The probability of  $SF$ ,  $P[SF]$ , is then evaluated by the inclusion-exclusion law of probability as

$$273 P[SF] = P[M_1] + P[M_2] - P[M_1 \cdot M_2] \quad (5)$$

274 Sampling  $N$  times the parameter space  $\mathbf{Y}$  yields

$$275 P[M_1] = P[Y_A] = N_A/N \quad (6)$$

$$276 P[M_2] = N_B/N \cdot P[h_{TR,j} > h_j] \quad (7)$$

277 Here,  $N_A$  and  $N_B$  indicate the number of sampling points in Region A and Region B, respectively. Since

278  $Y_A \cap Y_B = \emptyset$  (empty set),  $M_1$  and  $M_2$  do not overlap and

$$279 P[M_1 \cdot M_2] = 0 \quad (8)$$

280 Substituting (6) - (8) into (5) finally yields

$$281 P[SF] = \frac{N_A}{N} + \frac{N_B}{N} \cdot P[h_{TR,j} > h_j] \quad (9)$$

### 282 3.2 Computation of probabilities

283 To evaluate the probability of system failure (9), the methodology described below and shown in  
284 the flow chart depicted in Fig. 3 is then implemented.

- 285 (1) A number of  $N$  Monte Carlo realizations of  $\mathbf{Y}$ ,  $\mathbf{Y}_n$  (with  $n = 1, \dots, N$ ), characterized by a  
286 multivariate Gaussian distribution with mean  $\boldsymbol{\mu}$  and covariance  $\boldsymbol{\Sigma}$  estimated through a ML  
287 approach (see Section 2) is generated. For each  $\mathbf{Y}_n$ , the conductivity field,  $\mathbf{K}_n$ , is reconstructed  
288 in the study area according to the *CM* and *OC* model.
- 289 (2) The forward groundwater flow model is solved for all conductivity fields  $\mathbf{K}_n$  upon setting a  
290 flow rate equal to  $Q^{\min}$  in all pumping wells.



- 291 (3) As a result of step (2), Region A is identified. It includes the number of  $N_A$  realizations of  $\mathbf{K}$   
292 (and of  $\mathbf{Y}$ ) for which the  $SF$  is always detected.
- 293 (4) The forward groundwater flow model is solved for all conductivity fields  $\mathbf{K}_n$  not included in  
294 Region A upon setting a flow rate equal to  $Q^{\max}$  in all pumping wells.
- 295 (5) As a result of step (4), Region C is identified. It includes the number of  $N_C$  realizations of  $\mathbf{K}$   
296 (and of  $\mathbf{Y}$ ) for which the  $SF$  is never detected.
- 297 (6) As a result of steps (3) and (5), Region B is identified, which includes  $N_B = N - N_A - N_C$   
298 realizations of  $\mathbf{K}$ .
- 299 (7) Entries of vector  $\mathbf{Q}$  are considered independent and identically distributed (iid) random  
300 variables characterized by a uniform distribution within the support  $[Q^{\min}, Q^{\max}]$  and are  
301 sampled  $M$  times through a Latin Hypercube Sampling strategy.
- 302 (8) Groundwater flow simulations are run upon setting  $\mathbf{Q} = \mathbf{Q}_m$  ( $m = 1, \dots, M$ ) for all  $N_B$   
303 realizations of  $\mathbf{K}$  to evaluate the relative frequency corresponding to the number of realizations  
304 where (1) is satisfied.

305 This procedure requires performing  $2N$  (Steps 2 and 4) +  $N_B \times M$  (step 8) runs of the forward  
306 groundwater flow model for each conceptual model of the system. It can be remarked that the values of  
307  $N$  and  $M$  need to be sufficiently high to ensure stability in the computation of the target probabilities. In  
308 this context, note that relying on the full groundwater model set-up described in Section 2 to simulate  
309 hydraulic heads at the spring locations poses a significant challenge in terms of computational effort.  
310 For this reason, the target system response is evaluated upon relying on a surrogate (or reduced-order)  
311 model. For the purpose of our study, a surrogate model based on the generalized Polynomial Chaos  
312 Expansion (gPCE; e.g., Ghanem and Spanos, 1991; Xiu and Karniadakis, 2002; Le Maître and Knio,  
313 2010) is considered, the presented probabilistic risk assessment methodology being fully compatible

314 with other choices of model reduction techniques. Details about the methodology employed to obtain  
315 the surrogate model approximation are illustrated in Appendix B.

316 The framework of analysis is exemplified in Section 4 upon considering  $N_w = 5$  pumping wells  
317 located in the area with the highest spring density. The identifiers associated with these wells are (from  
318 North to South): Arzago, Misano, Capralba, Sergnano, and Spino. The hydraulic head constraint  
319 expressed by (1) is applied to  $N_s = 34$  natural springs located in the proximity of these wells. The  
320 location of the pumping wells and of the springs is depicted in Fig. 1b. The flow rate  $Q_w$  ( $w = 1, \dots, 5$ )  
321 of each well is allowed to vary between  $Q^{\min} = 0$  and  $Q^{\max} = 0.9 \text{ m}^3/\text{sec}$ . This range of values has been  
322 selected upon considering that the total amount of water withdrawn from these wells in the calibrated  
323 models (see Section 4 and Appendix A) is  $1.18 \text{ m}^3/\text{s}$  (corresponding to  $3.72 \times 10^7 \text{ m}^3/\text{year}$ ) and with the  
324 aim of including in the analysis also scenarios mimicking a significant increase of groundwater  
325 withdrawal from the aquifer. A minimum flow rate  $Q_s^{\min} = 0.097 \text{ m}^3/\text{s}$  is set at each spring. This value  
326 ensures a minimum value for the total spring flow rate equal to  $3.31 \text{ m}^3/\text{s}$ . The latter corresponds to a  
327 decrease of 25 % with respect to the value employed in the calibrated models, i.e.,  $4.42 \text{ m}^3/\text{s}$  (see  
328 Section 4 and Appendix A).

#### 329 **4. Results and discussion**

330 Values of ML estimates ( $\mu$ ) of facies log-conductivities as well as a the posterior covariance  
331 matrix ( $\Sigma$ ) of the corresponding estimation error are listed in Table 2 for the two conceptual models  
332 considered. Figure 4 compares the prior (Uniform) probability density functions (see Appendix A,  
333 Table A.1), *pdf*, of each parameter against their (marginal, Gaussian) posterior counterparts stemming  
334 from model calibration. ML conductivity estimates are consistent with the nature of the geomaterials  
335 with which they are associated, lowest and largest values being referred to clay (Facies 1) and gravel  
336 and fractured conglomerate (Facies 2 and 3), respectively. The uncertainty related to these estimates (as

337 quantified in terms of the diagonal entries of  $\Sigma$ ) is (at least) one order of magnitude smaller than the  
338 (prior) uncertainty corresponding to each parameter (as quantified through the variance of the prior  
339 *pdf*), in line with the ability of hydraulic head data to increase our level of knowledge of hydraulic  
340 parameters of the geomaterials contributing to internal make-up of the system.

341 The spatial distribution of hydraulic heads computed with the calibrated *CM* and *OC* models is  
342 depicted in Fig. 1b. The main flow direction is from North to South, the hydraulic gradient decreasing  
343 mildly along this direction, with a mean value of approximately 3.7%. One can note that both  
344 calibrated models yield essentially the same overall distribution of hydraulic heads, an observation  
345 which is also supported by the results shown in Appendix A and related to the ability of the calibrated  
346 models to reproduce the observed heads (see scatterplot in Figure A.2) as well as the mean annual total  
347 discharge at the natural springs (see Appendix A).

348 Following the workflow described in Section 3.2 and in Fig. 3, the probabilities  $P[Y_A]$ ,  $P[Y_C]$ , and  
349  $P[Y_B]=1-P[Y_A]-P[Y_C]$  are computed. This is accomplished upon relying on a sample of  $N = 10^4$   
350 realizations of  $\mathbf{K}$  which enables one to obtain stable evaluation of the quantities of interest (details not  
351 shown). Values  $P[Y_A] = 38.4\%$ ,  $P[Y_B] = 46.5\%$ , and  $P[Y_C] = 15.1\%$  for *CM*; and  $P[Y_A] = 33.7\%$ ,  $P[Y_B]$   
352  $= 32.4\%$ , and  $P[Y_C] = 33.9\%$  for *OC* are obtained in our scenarios. The resulting Regions A, B and C  
353 are depicted in Fig. 5 across the considered parameter spaces for *CM* (Fig 5a) and *OC* (Fig. 5b). One  
354 can note that the two modeling approaches yield similar values of  $P[Y_A]$ , i.e., the probability that a  
355 scenario falls within the region where the desired constraints cannot be satisfied. Conversely, the  
356 choice of the conceptual model strongly affects  $P[Y_C]$  (and therefore  $P[Y_B]$ ), a higher probability to be  
357 in Region C (where *SF* is never detected) being observed for *OC* than for *CM*. This result is related to  
358 the observation that the uncertainty in the conductivity field may have a different impact on the  
359 variability of hydraulic heads depending on the conceptual model adopted. In this sense, it is noted that  
360 local sharp changes of hydraulic conductivity can occur in *CM*, while *OC* leads to a smoother spatial

361 variation of conductivity. Therefore, *CM* is (in general) characterized by spatial variations of the  
362 hydraulic gradient that are larger than the ones observed in *OC*, yielding a higher probability in *CM*  
363 than in *OC* that a given conductivity realization be associated with Region C. In this context, the results  
364 related to the *CM* model can be viewed as more conservative than those linked to *OC* for the purpose of  
365 the risk analysis here considered.

366 The overall probability of system failure,  $P[SF]$ , evaluated according to (9) and considering  $M =$   
367  $10^5$  random realizations of well flow rates,  $\mathbf{Q}_m$  ( $m = 1, \dots, M$ ), is depicted in Fig. 6 as a function of the  
368 total (normalized) volume of water withdrawn from the aquifer per unit time by the system of pumping  
369 wells,  $Q_T^* = \sum_{w=1}^{N_w} Q_w / Q_{\max}$ . Relying on  $M = 10^5$  enable one to investigate the system behavior for a  
370 sufficiently high number of combinations of flow rates at the five investigated wells. The variability of  
371  $P[SF]$  associated with a given value of  $Q_T^*$  in Fig. 6 is related to the way  $Q_T^*$  is partitioned amongst the  
372 wells and its analysis enables one to quantify the influence of such a partitioning on  $P[SF]$ . It is noted  
373 that the impact of the flow rate distribution amongst the wells is larger in *CM* than in *OC*. For each  
374 modeling approach, the lower bound of the cloud of points in Fig. 6 leads to identifying the best trade-  
375 off between the need to maximize the benefit associated with water withdrawal from the aquifer while  
376 minimizing  $P[SF]$ . As such, it can be identified as a Pareto front, collecting the solutions for which an  
377 improvement to a given objective (corresponding to maximizing  $Q_T^*$  in our example) is not possible  
378 without a reduction in the possibility of achieving another objective, i.e., here represented by the  
379 minimization of  $P[SF]$  (Deb et al., 2002). These results are based on specific definitions of system  
380 failure, design variables, scenarios and sources of uncertainty. In this context, the evaluation of the  
381 probability of system failure provides a quantitative basis which one can then envision to include as a  
382 tool in a decision support system in the framework of groundwater resources management and  
383 protection. While costs associated with alternative exploitation strategies are not explicitly considered

384 in this study, these can be accounted for in a cost-benefit analysis for which our risk assessment  
385 provides input. All of these elements underpin the results of probabilistic risk analyses and would  
386 benefit from a continuous update and refinement stemming from a participatory process and feedback  
387 with policy makers, local authorities, and stakeholders.

388 Figure 7a depicts the total normalized flow rate as a function of  $P[SF]$  for some selected points at  
389 the Pareto front. Corresponding distribution of optimal normalized flow rates,  $Q_w^* = Q_w / Q^{\max}$ , for each  
390 of the five wells considered in the analysis are depicted in Figs. 8b and 8c for *CM* and *OC*,  
391 respectively. A conceptualization of the subsurface system based on *OC* leads to the possibility of  
392 extracting an increased water volume from the aquifer with respect to *CM* for a given value of  $P[SF]$ .  
393 This is consistent with the observation that  $P[Y_C]$  is smaller for *CM* than for *OC*, as noted above. For  
394 both modeling approaches it can be noted that the optimal total flow rate increases almost linearly with  
395  $P[SF]$  (see Fig. 7a). Otherwise, a non-linear trend is observed when plotting the values of the  
396 normalized optimal well rates at each well versus  $P[SF]$  (Figs. 7b-c), possibly due to local effects. For  
397 example, the rate of increase of optimal pumping rate with  $P[SF]$  at the Misano well for *CM* is very  
398 low in the interval  $0.45 < P[SF] < 0.65$  and sharply increases for  $P[SF] > 0.70$  (see Fig. 7b). When  
399 considering the *OC* model, the optimum values of the pumping rates at the Spino and Arzago wells are  
400 close to the upper bound of the assigned range of variability for e.g.  $0.55 < P[SF] < 0.65$ . This result is  
401 associated with the values of hydraulic head thresholds that have been imposed at the springs closest to  
402 these wells.

403 The analyses illustrated above do not enable one to identify the most vulnerable spring of the  
404 system because of the way  $SF$  is defined in our application example, i.e., the depletion of at least one  
405 spring. In the context of environmental applications, such a choice is grounded on the interest in  
406 considering the most conservative scenario and guaranteeing a minimum flow rate for each spring in  
407 the system, as compatible with environmental requirements. Otherwise, one could also be interested in

408 assessing which amongst the springs in the system would be associated with the highest risk of  
409 depletion, depending on the adopted pumping scheme. This issue is addressed upon evaluating the  
410 relative frequency of spring depletion considering various pumping schemes. The probability of failure  
411 for the  $j$ -th spring ( $P[SpF_j]; j = 1, \dots, 34$ ) is evaluated as the number of times the constraint (1) is not  
412 satisfied across the collection of  $N = 10^4$  realizations of  $\mathbf{K}$ . As an example of the results one can obtain,  
413 the case at the Pareto front associated with Fig. 7b-c and  $P[SF] = 0.45$  is considered. The (normalized)  
414 flow rate for each well in the system (one well at a time) is then varied between 0 and 1, while fixing  
415 the remaining four extracted rates at their optimal values (represented in Fig. 7b-c). Results of this  
416 analysis are depicted in Figs. 8 and 9 for *CM* and *OC*, respectively. In order to streamline the analysis,  
417 the 34 springs in the area are organized into 5 groups, according to the closest well. The group of springs  
418 associated with the well whose flow rate is varied in this analysis is identified with a red bracket in the  
419 various panels of Figs. 8 and 9. As expected, for both modeling approaches it is observed that  
420 increasing the flow rate at a given well mainly affects  $P[SpF_j]$  at the subset of springs located in its  
421 proximity (and demarcated by the red bracket). In particular, the Spino well can only affect the value of  
422  $P[SpF_j]$  at the corresponding group of springs for both *CM* and *OC* (see Figs. 8e and 9e). This finding  
423 is consistent with the observation that this well is quite isolated with respect to the others (see Fig. 1b).  
424 Note that each of the springs within a given group is characterized by a unique behavior in terms of  
425  $P[SpF_j]$ , which is associated with the risk of depletion for increasing pumping rates of the closest well.  
426 Similar results have been obtained for  $P[SF] > 0.45$  (not shown). For completeness, a statistical  
427 analysis of hydraulic head evaluated at all spring locations corresponding to the pumping scheme of  
428 Fig. 7b-c and  $P[SF] = 0.45$  is provided as Supplementary Data.

## 429 5. Conclusions

430 Our study provides methodological advancements by proposing a novel approach for  
431 Probabilistic Risk Assessment (PRA) targeting reduction of the flow rate at natural springs due to

432 excessive aquifer exploitation for supply or productive use. The approach and ensuing operational  
433 workflow are exemplified considering a three-dimensional, large scale aquifer system whose  
434 characterization is fraught by elements of uncertainty related to the possibility of representing the  
435 subsurface through diverse conceptual geological models, each associated with uncertain hydraulic  
436 parameters. The level of knowledge of the latter is conditioned to available hydraulic head information  
437 through a Maximum Likelihood inverse modeling approach. Our analysis explicitly includes the impact  
438 of model and associated parameter uncertainty on the evaluation of the probability of system failure.  
439 The latter is quantified through the constrain that hydraulic head of a target set of active springs does  
440 not fall below a given threshold value as a consequence of groundwater pumping.

441 The application of the approach we present to the investigated field site leads to the following  
442 major conclusions.

- 443 1. The choice of the conceptual model employed to characterize the internal geological makeup of  
444 the groundwater system strongly affects probability of system failure. While the scenario  
445 corresponding to conceptual geological model based on a composite medium (*CM*) approach  
446 yields locally sharp changes of hydraulic conductivity (and therefore of hydraulic head  
447 gradients), the setting corresponding to an overlapping continua (*OC*) approach leads to  
448 smoother spatial variations of these quantities. As a consequence, uncertainties associated with  
449 the ensuing conductivity fields, even as constrained through model calibration, has a different  
450 impact on the variability of hydraulic heads depending on the conceptual model adopted.
- 451 2. Our methodology enables one to include uncertainty in model parameters which is  
452 constrained by available hydraulic head information through a Maximum Likelihood inverse  
453 modeling approach. This element provides a marked interconnection between the processes  
454 of model calibration and the use of a given model for predictions of the system response due  
455 to possible changes in the forcing terms.

- 456 3. For a given groundwater withdrawal, probability of system failure is smaller for the overlapping  
457 continua than for the composite medium approach. As such, the latter scenario can be viewed as  
458 more conservative than its counterpart based on the overlapping continua concept for the  
459 purpose of the probabilistic analysis here considered.
- 460 4. Our operational workflow conducive to the Probabilistic Risk Assessment of natural springs  
461 under uncertainty makes effective use of a combination of Fault Tree Analysis, inverse  
462 modeling of a large scale groundwater flow system, development of a surrogate groundwater  
463 flow model, and uncertainty quantification to evaluate the probability that the functioning of the  
464 system considered attains a critical state. The proposed methodology allows assessing the best  
465 compromise between two conflicting objectives, corresponding to (i) the minimization of  
466 probability of system failure and (ii) the possibility to guarantee significant groundwater  
467 extraction rates, with the aim of identifying the optimal total flow rate as well as its optimal  
468 distribution amongst operating pumping wells. The structure of the methodology renders it  
469 amenable to be effectively included in a decision support system for groundwater resources  
470 management and exploitation.

## 471 472 **6. Appendix**

### 473 **Appendix A – Model calibration**

474 For each conceptual model, estimates of facies log-conductivities,  $Y_i = \log k_i$  ( $i = 1, \dots, N_p$ ), and of  
475 the leakage coefficient,  $l_d$ , have been obtained through an inverse modeling approach upon relying on  
476 a Maximum Likelihood (ML) framework (see e.g., Carrera and Neumann, 1986; Poeter and Hill, 1997;  
477 Tarantola, 2005; Carrera et al., 2005; Chavent, 2010).



478 The level of knowledge of the uncertain hydraulic parameters is conditioned to available  
479 hydraulic head information through a Maximum Likelihood inverse modeling approach. Let  $N_p$  and  $N_h$   
480 be the number of unknown model parameters and hydraulic head measurements, respectively. The  
481 vector of unknown model parameters,  $\mathbf{p} = [p_1, p_2, \dots, p_{N_p}]$ , the vector of hydraulic head measurements,  
482  $\mathbf{h}^* = [h_1^*, h_2^*, \dots, h_{N_h}^*]$ , the vector of model predictions,  $\hat{\mathbf{h}} = [\hat{h}_1, \hat{h}_2, \dots, \hat{h}_{N_h}]$ , and the prior covariance  
483 matrix of the head measurement errors,  $\mathbf{C}_h$ , are then introduced. As commonly assumed (e.g., Carrera  
484 and Neuman, 1986), errors  $h_i^*$  are considered to be uncorrelated. This renders  $\mathbf{C}_h = \sigma_h^2 \mathbf{V}_h$  diagonal  
485 with the nonzero terms equal to the head observation error variance,  $\sigma_h^2$ .

486 The Maximum Likelihood (ML) estimate,  $\hat{\mathbf{p}}$ , of  $\mathbf{p}$  is obtained through minimization of the  
487 negative log likelihood criterion (e.g., Carrera and Neumann, 1986; Bentley, 1993; Poeter and Hill,  
488 1997; Tarantola, 2005; Carrera et al., 2005; Chavent, 2010)

$$489 \quad NLL = \sum_i^{N_h} \frac{J_i}{\sigma_h^2} + \ln |\mathbf{C}_h| + N_h \ln(2\pi) \quad (10)$$

490 with respect to  $\mathbf{p}$ . The quantity  $J_i$  in Eq. (10) is defined as the squared difference between measured and  
491 predicted hydraulic heads

$$492 \quad J_i = (h_i^* - \hat{h}_i)^2. \quad (11)$$

493 Considering  $\sigma_h^2$  as a constant, minimizing  $NLL$  (for fixed  $N_h$ ) is tantamount to minimizing the  
494 least square criterion

$$495 \quad J = \sum_{i=1}^{N_h} (h_i^* - \hat{h}_i)^2 \quad (12)$$

496 Minimization of Eq. (12) is performed upon relying on the iterative Levenberg-Marquardt  
 497 algorithm implemented in the public domain code PEST (Doerthy, 2018). Then, the ML estimate of  
 498  $\sigma_h^2$  is given by

$$499 \quad \hat{\sigma}_h^2 = \frac{J_{\min}}{N_h} \quad (13)$$

500 where  $J_{\min}$  is the minimum of  $J$ .

501 The posterior estimation error covariance matrix,  $\Sigma$ , is a measure of the quality of parameter  
 502 estimates conditioned to available hydraulic head information and is estimated as (Carrera and  
 503 Neuman, 1986)

$$504 \quad \Sigma = \hat{\sigma}_h^2 [\mathbf{S}^T \mathbf{V}_h^{-1} \mathbf{S}]^{-1}. \quad (14)$$

505 Here,  $\mathbf{S}$  is the Jacobian (sensitivity) matrix, whose components are  $\partial h_r / \partial p_i$  with ( $r = 1, \dots, N_h$ ; and  $i =$   
 506  $1, \dots, N_p$ ).

507 As calibration data, we consider yearly-averaged hydraulic heads collected at 35 observation  
 508 wells during year 2015 and mean annual total discharge monitored at the springs,  $Q_{sp}$ . Location of  
 509 monitoring wells and springs is depicted in Fig. 1b. Details about available data are offered in Bianchi  
 510 Janetti et al. (2019). Lower and upper bounds assigned to  $Y_i$  prior to model calibrations are based on  
 511 typical values of hydraulic conductivities characterizing each of the identified geomaterials (see Table  
 512 A.1).

513 Calibration of model parameters has been performed using the following iterative procedure:

- 514 *i)* Facies log-conductivity values,  $Y_i$ , are estimated considering the available hydraulic  
 515 head measurements and a first tentative value for the leakage coefficient,  $l_d$ ;
- 516 *ii)* An estimate of  $l_d$  is obtained by considering available data about  $Q_{sp}$  while setting  
 517 hydraulic conductivities at the optimal values obtained at step (*i*);

518 *iii)* Values of  $Y_i$  are subject to a further estimation process while setting  $l_d$  at the value  
519 resulting from step *(ii)* and are then compared against the values obtained at step *(i)*.

520 Convergence of the procedure requires only a few iterations, leading to optimal values of  $Y_i$  and  
521  $l_d$  obtained on the basis of both hydraulic head and spring flow rate measurements. Estimated values of  
522  $l_d$  are  $1.21 \times 10^{-6} \text{ s}^{-1}$  and  $1.30 \times 10^{-6} \text{ s}^{-1}$  for *CM* and *OC*, respectively.

523 Figure A.2 depicts scatterplots of simulated versus observed hydraulic heads at the available  
524 monitoring stations for *CM* (Fig. A.1a) and *OC* (Fig. A.1b). These results suggest that both calibrated  
525 models can accurately reproduce available hydraulic head observations at the site. Groundwater levels  
526 obtained for each spring location in the two calibrated models are depicted in Figure A.2.

## 527 **Appendix B – Surrogate model**

528 The uncertain model inputs are here associated with *(a)* flow rates  $Q_w$  (with  $w = N_w$ ) related to the  
529 pumping wells considered in the analysis and *(b)* facies log-conductivities ( $Y_i$ , with  $i = n_f$ ). Uncertain  
530 parameters are collected in a vector  $\mathbf{p} = [\mathbf{Q}, \mathbf{Y}]$  of dimension  $D = N_w + N_p$ . For the purpose of  
531 evaluating the surrogate model, we consider the entries of  $\mathbf{Q}$  and  $\mathbf{Y}$  as independent and identically  
532 distributed (iid) random variables, each characterized by a uniform density. The (random) parameter  
533 space across which the full system model is evaluated and the surrogate model is constructed is then  
534 defined as  $\Gamma = [\mathbf{p}^{\min}, \mathbf{p}^{\max}]$ ,  $\mathbf{p}^{\min}$  and  $\mathbf{p}^{\max}$  denoting vectors containing lower and upper bounds of  
535 parameter variability intervals, respectively (see Table A.1). We set  $Q_w^{\min} = 0$  and  $Q_w^{\max} = 0.9 \text{ m}^3 \text{ s}^{-1}$  for  
536 all wells, according to the scenarios described in Section 3.2. The choice of  $Y_i^{\min}$  and  $Y_i^{\max}$  is based on  
537 typical hydraulic characteristics of each of the identified geomaterials (see Fig. 4 and Table A.1). As  
538 stated in Section 3.2, our surrogate (or reduced-order) model relies on the generalized Polynomial  
539 Chaos Expansion (gPCE; e.g., Ghanem and Spanos, 1991; Xiu and Karniadakis, 2002; Le Maître and

540 Knio, 2010). We then approximate  $h_j(\mathbf{Q}, \mathbf{Y})$  in Eq. (1) through a linear combination of multivariate  
 541 orthonormal Legendre polynomials, i.e.,  $\psi_{\mathbf{x}}(\mathbf{p})$ , as

$$\begin{aligned}
 f(\mathbf{p}) &\cong f_0 + \sum_{i=1}^D \sum_{\mathbf{x} \in \mathfrak{S}_i} \beta_{\mathbf{x}} \psi_{\mathbf{x}}(\mathbf{p}) + \sum_{i=1}^D \sum_{j=1}^D \sum_{\mathbf{x} \in \mathfrak{S}_{i,j}} \beta_{\mathbf{x}} \psi_{\mathbf{x}}(\mathbf{p}) + \dots; \\
 \psi_{\mathbf{x}}(\mathbf{p}) &= \prod_{i=1}^D \psi_{i,x_i}(p_i); \quad \beta_{\mathbf{x}} = \int_{\Gamma} f(\mathbf{p}) \psi_{\mathbf{x}}(\mathbf{p}) \rho_{\Gamma_{\mathbf{p}}} d\mathbf{p},
 \end{aligned}
 \tag{15}$$

543 where  $\mathbf{x} = \{x_1, \dots, x_M\} \in \mathbb{N}^M$  is a multi-index expressing the degree of each univariate polynomial,  
 544  $\psi_{i,x_i}(p_i)$ ;  $\beta_{\mathbf{x}}$  are the gPCE coefficients;  $\rho_{\Gamma_{\mathbf{p}}}$  denotes the *pdf* of  $\mathbf{p}$ ;  $\mathfrak{S}_i$  and  $\mathfrak{S}_{i,j}$  include all indices such  
 545 that only the  $i$ -th component does not vanish or only the  $i$ -th and  $j$ -th components are not zero,  
 546 respectively, and so on. Evaluating coefficients  $\beta_{\mathbf{x}}$  in Eq. (15) entails resorting to a regression-based  
 547 method (Sudret, 2008). The latter is based on (a) the evaluation of the full model and its gPCE  
 548 approximation at a number of points in the parameter space and (b) the minimization of the sum of the  
 549 square of the differences between the exact and the approximated solutions. Here, accurate results have  
 550 been obtained truncating the gPCE at order 3, requiring  $N_t = 1115$  and 720 full model runs for *CM* and  
 551 *OC*, respectively (due to the different number of input parameters) which are performed using a quasi-  
 552 Monte Carlo sampling technique (see e.g., Feil et al., 2009; Fajraoui et al., 2012; Maina and  
 553 Guadagnini, 2018). The ability of a gPCE of a given order to approximate hydraulic heads at the target  
 554 points (i.e., locations corresponding to the springs) is assessed upon considering the full model  
 555 solutions evaluated at  $N_V = 100$  sets of parameter values, randomly selected in the parameter space and  
 556 not employed for the assessment of the gPCE. Figure B.1 depicts scatterplots of  $h_{gPCE,j,k}$  versus  $h_{j,k}$   
 557 computed for the two conceptual models considered at all target points  $j$  (corresponding with the 34  
 558 spring locations introduced in Section 3.2) for all  $N_V$  sets. This figure clearly shows a good agreement

559 between  $h_{j,k}$  and  $h_{gPCE,j,k}$ . We also computed a mean absolute relative error ( $MARE_j$ ) between the full  
560 model and the gPCE approximation for each spring location, i.e.,

$$561 \quad MARE_j = \frac{1}{N_V} \sum_{k=1}^{N_V} \frac{|h_{j,k} - h_{gPCE,j,k}|}{h_{j,k}} \quad j = 1, \dots, N_s \quad (16)$$

562 Average values of this metric, evaluated across the set of  $N_s$  spring locations, are 0.017 % and 0.035 %  
563 for *CM* and *OC*, respectively. These results suggest that the considered surrogate models enables us to  
564 capture with high fidelity the full model results needed for the purpose of our analysis.

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## Tables

**Table 1.** List of the  $n_f = 5$  facies (or geomaterial classes) identified in the study area, together with their volumetric fraction.

$M_i$	Description	$f_i$ (%)
1	Clay and silt	36.77
2	Gravel, sand and gravel	32.92
3	Fractured conglomerate	10.64
4	Compact conglomerate, sandstone	14.94
5	Fine and silty sand	4.73

**Table 2.** Statistical parameters of the multivariate normal distributions considered in the analysis.

Groundwater Model	ML estimates	Estimation error covariance matrix
$CM$	$\boldsymbol{\mu} = [-4.39, -1.67, -1.92]$	$\boldsymbol{\Sigma} = \begin{bmatrix} 1.62 \times 10^{-3} & -2.57 \times 10^{-3} & 4.90 \times 10^{-3} \\ \dots & 3.63 \times 10^{-2} & -1.40 \times 10^{-2} \\ \dots & \dots & 2.65 \times 10^{-2} \end{bmatrix}$
$OC$	$\boldsymbol{\mu} = [-1.74, -2.00]$	$\boldsymbol{\Sigma} = \begin{bmatrix} 2.60 \times 10^{-2} & 2.07 \times 10^{-2} \\ \dots & 6.07 \times 10^{-2} \end{bmatrix}$

## Appendix

**Table A.1.** Selected uncertain model inputs and associated intervals of variability, as defined by their lower (min) and upper (max) boundaries.

<b>Parameter</b>	<b>Description</b>	<b>Min</b>	<b>Max</b>
$p_w$ (m <sup>3</sup> /s) with $w=1,\dots,5$	Pumping rate at well $w$ , $Q_w$	0	0.9
$\text{Log } p_6$ (m/s)	Log-conductivity of facies 1, $Y_1$	-5.5	-3.5
$\text{Log } p_7$ (m/s)	Log-conductivity of facies 2, $Y_2$	-3	-1
$\text{Log } p_8$ (m/s)	Log-conductivity of facies 3, $Y_3$	-2.5	-0.5

## Figures

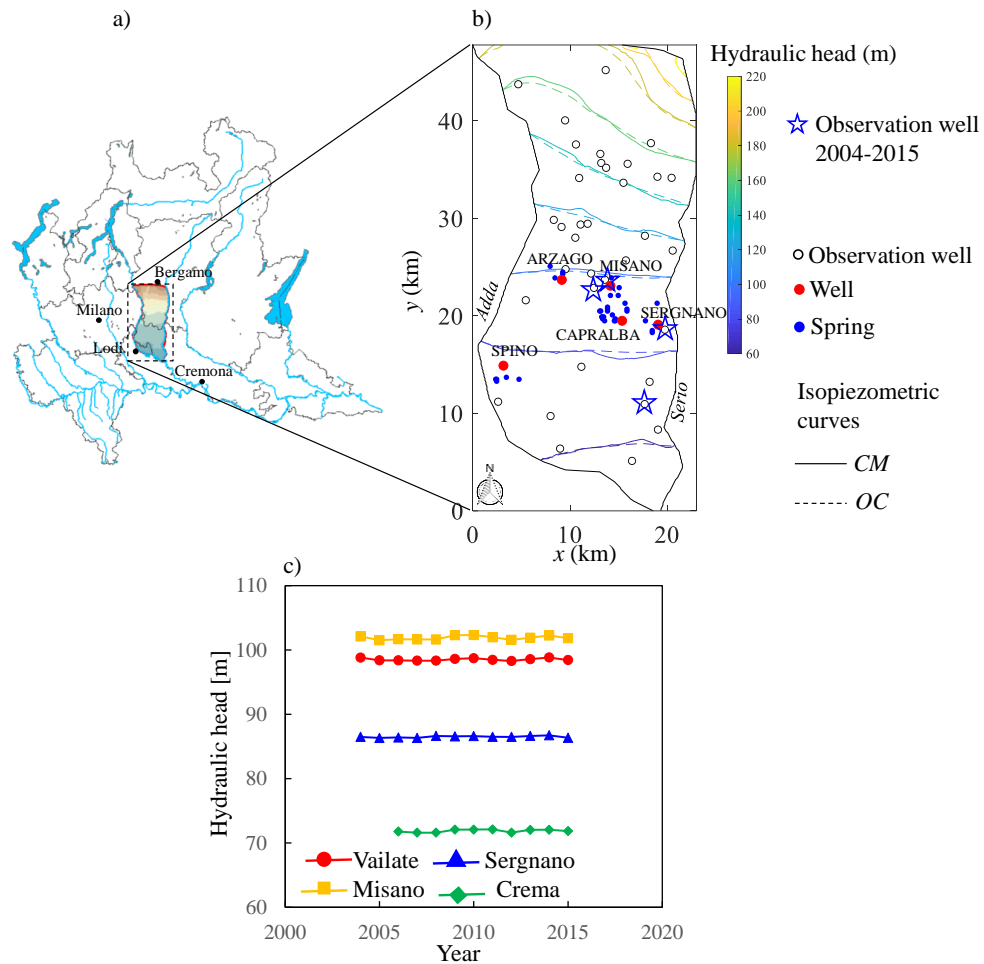


Figure 1. Location of (a) the study area (shaded zone) within the Po Plain (Northern Italy), (b) springs, pumping and observation wells considered in the analysis; hydraulic head distributions of the calibrated models are also shown, continuous and dashed curves being associated with the *Composite Medium* (CM) and the *Overlapping Continua* (OC) conceptual model, respectively; (c) yearly-averaged hydraulic head (years 2004 to 2015) at four observation wells (Vailate, Sergnano, Misano, and Crema) used in the model calibration process (locations of these observation wells within the study area (b) are identified with stars).

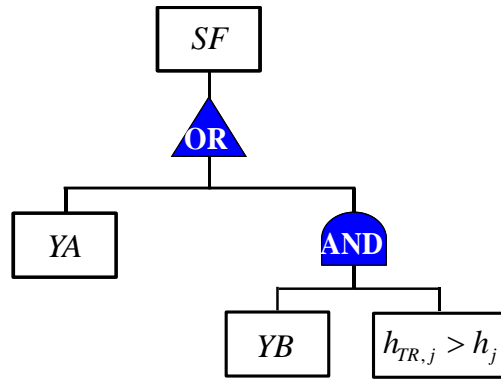


Figure 2. Fault tree leading to system failure (*SF*).

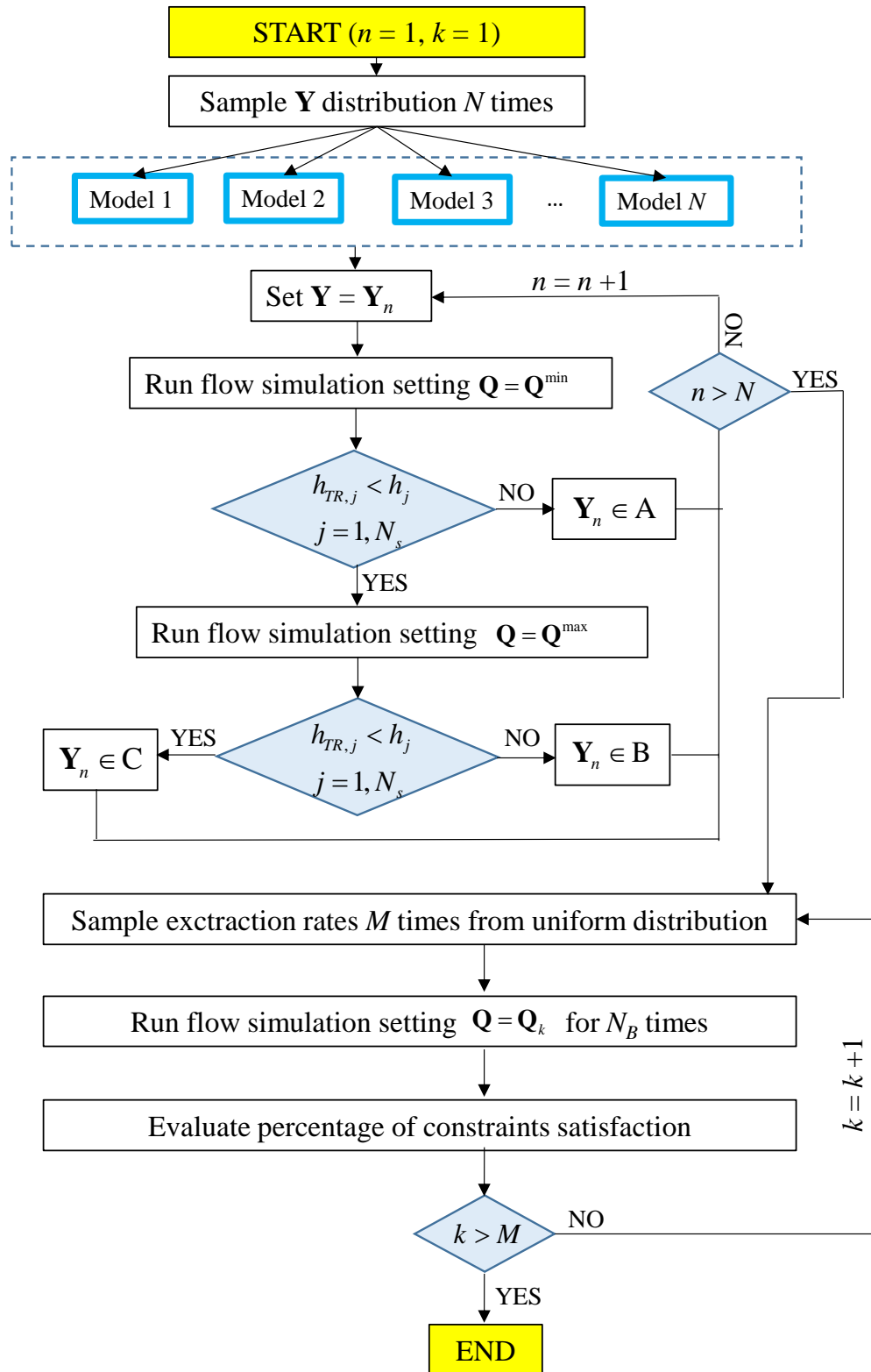


Figure 3. Workflow of the proposed methodology.

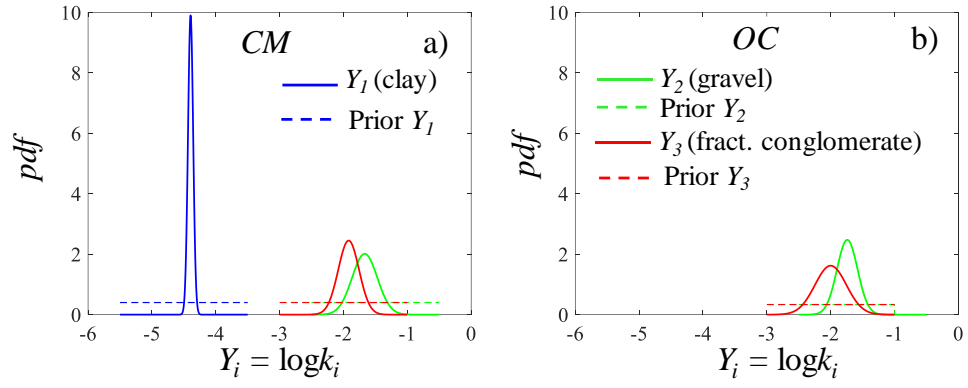


Figure 4. Marginal prior (dashed) and posterior (solid) *pdf* of facies log-conductivities for the (a) *Composite Medium (CM)* and (b) *Overlapping Continua (OC)* conceptual modeling approaches.



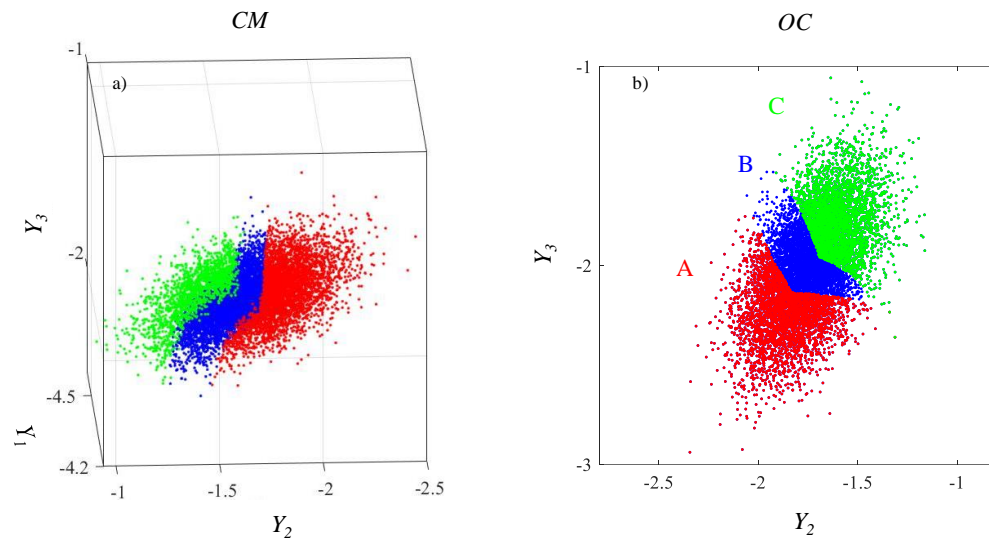


Figure 5. Identification of Region A (red), B (blue), and C (green) across the parameter space for the (a) *Composite Medium (CM)* and (b) *Overlapping Continua (OC)* conceptual modeling approaches.

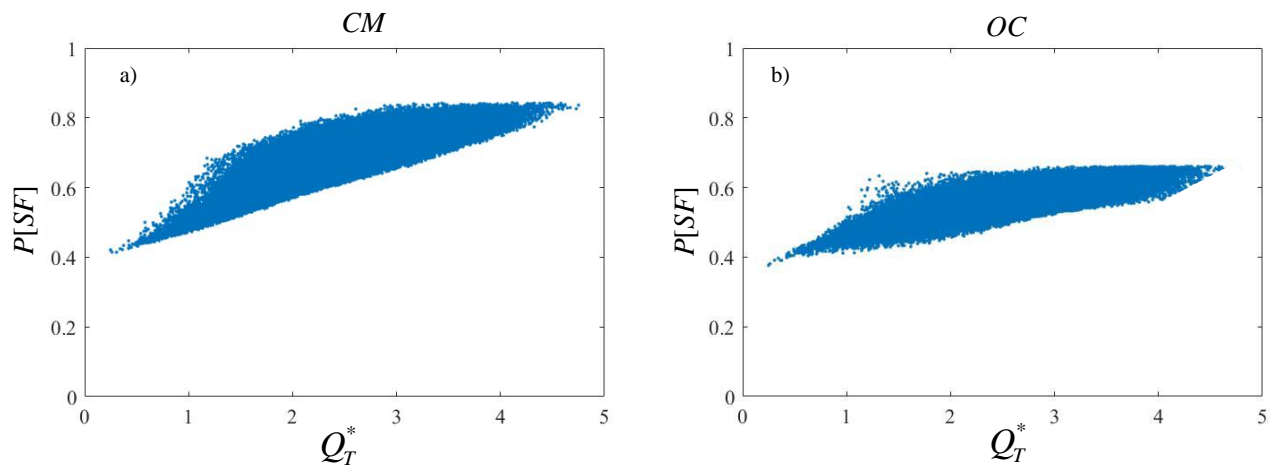


Figure 6. Probability of system failure ( $P[SF]$ ) as a function of the total (normalized) rate extracted from the aquifer for the (a) *Composite Medium (CM)* and (b) *Overlapping Continua (OC)* conceptual modeling approaches.

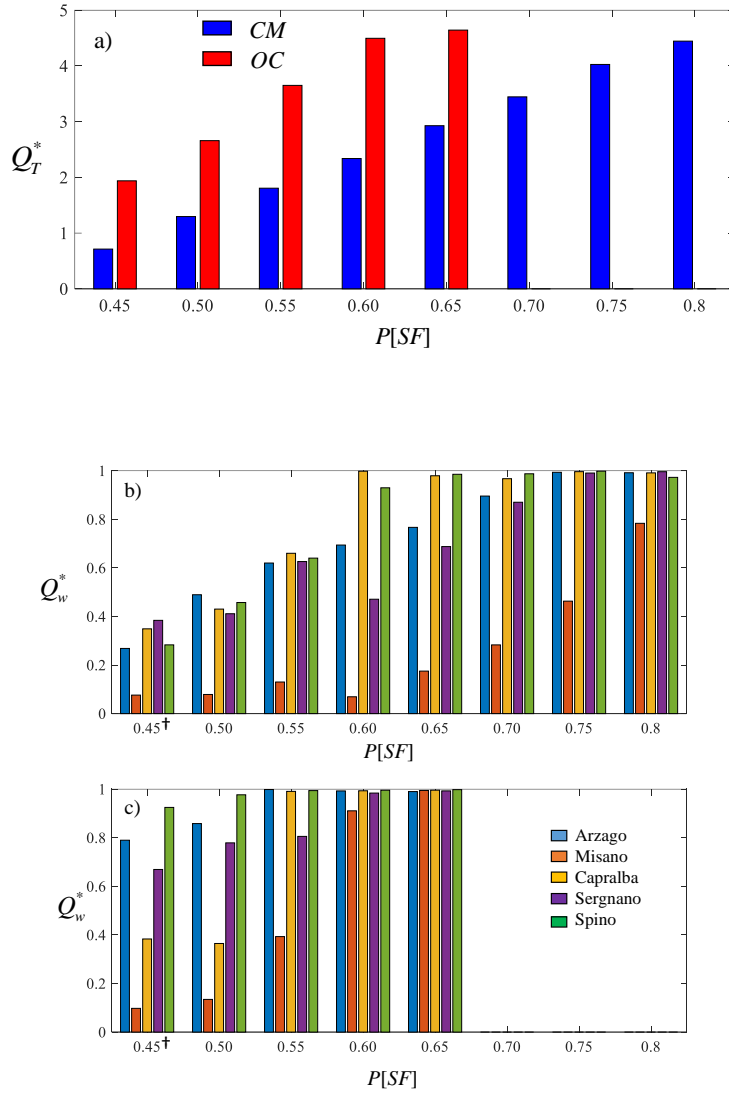


Figure 7. (a) Total flow rate versus  $P[Sf]$  for some selected points at the Pareto front of Fig. 7 for the *Composite Medium (CM)* and *Overlapping Continua (OC)* modeling approaches; and corresponding optimal normalized flow rate computed for each pumping well for (b) *CM* and (c) *OC*. The symbol † denotes the set of flow rates considered for the analysis shown in Figs. 8 and 9.

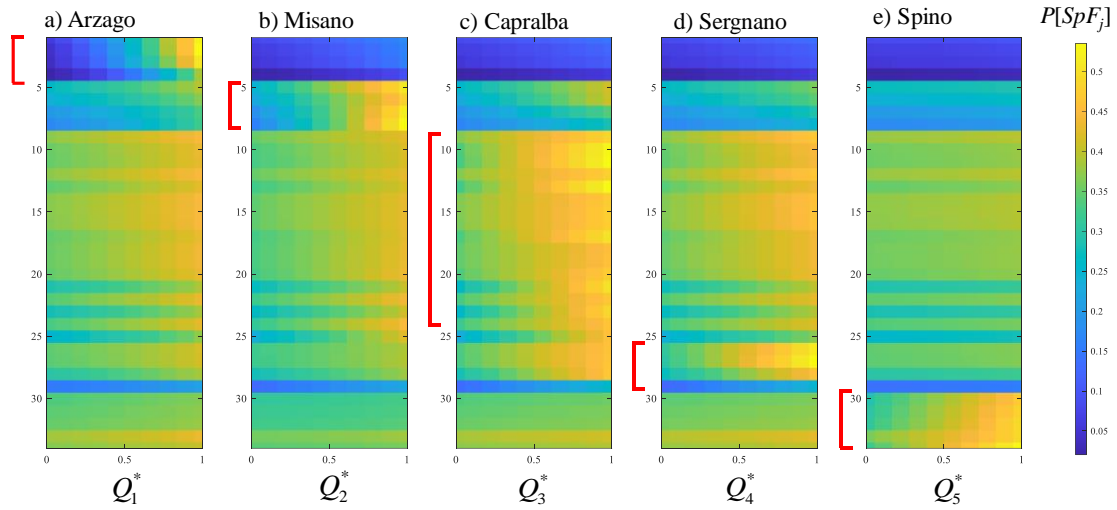


Figure 8. Probability that system failure takes places at the  $j$ -th spring ( $P[SpF_j]; j = 1, \dots, 34$ ) evaluated upon varying the (normalized) flow rate at a single well  $Q_w^*$  (with  $w = 1$  in (a), 2 in (b), 3 in (c), 4 in (d) and 5 in (e)), while keeping the remaining four extracted rates at their optimal values (represented in Fig. 7b-c and corresponding to  $P[SF] = 0.45$ ). Brackets identify the group of springs closest to the well whose flow rate is varied. Results are associated with the *Composite Medium (CM)* modeling approach.

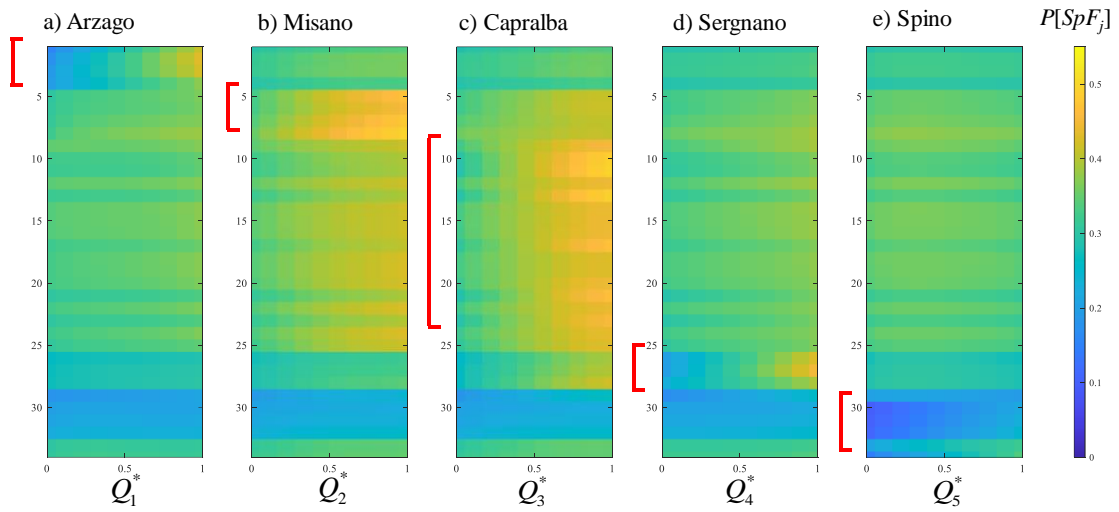


Figure 9. Probability that system failure takes places at the  $j$ -th spring ( $P[SpF_j]; j = 1, \dots, 34$ ) evaluated upon varying the (normalized) flow rate at a single well  $Q_w^*$  (with  $w = 1$  in (a), 2 in (b), 3 in (c), 4 in (d) and 5 in (e)), while keeping the remaining four extracted rates at their optimal values (represented in Fig. 7b-c and corresponding to  $P[SF] = 0.45$ ). Results are associated with the *Overlapping Continua (OC)* modeling approach.

Appendix A

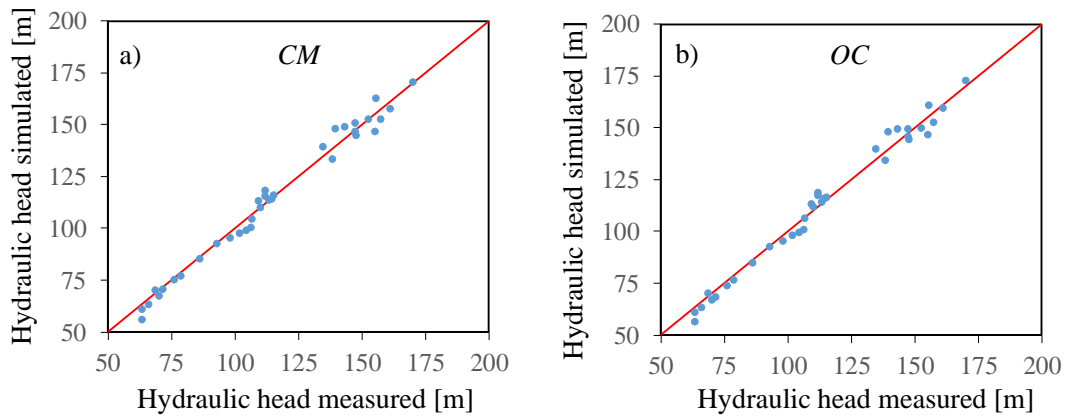


Figure A.1. Simulated versus measured hydraulic heads at observation well locations for the (a) *Composite Medium (CM)* and (b) *Overlapping Continua (OC)* conceptual modeling approaches.

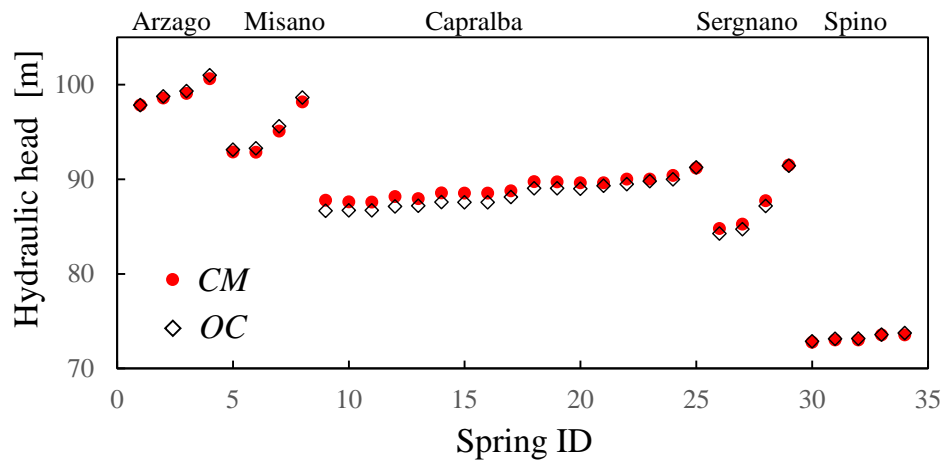


Figure A.2. Simulated hydraulic heads at spring locations for the (a) *Composite Medium* (CM; circle) and the (b) *Overlapping Continua* (OC; diamond) conceptual modeling approaches.

## Appendix B

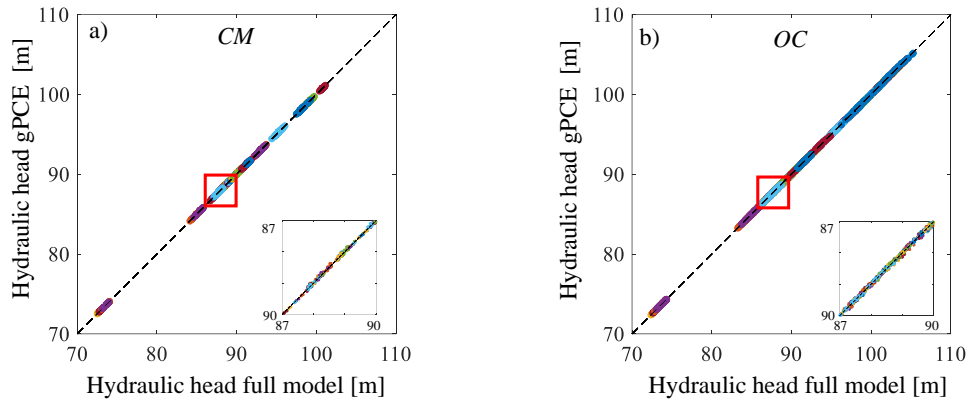


Figure B.1. Head at spring locations evaluated through the generalized Polynomial Chaos Expansion, gPCE, surrogate model versus their counterparts computed with the full model for the  $N_V = 100$  sets of parameter values randomly selected in the parameter space and not employed for the assessment of the gPCE for the (a) *Composite Medium (CM)* and (b) *Overlapping Continua (OC)* conceptual modeling approaches. Results for each spring location are reported with different colors. The two embedded panels represent a zoom on the region highlighted in red for the two modeling approaches.



**Supplementary material for on-line publication only**

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## **Credit author statement**

Emanuela Bianchi Janetti: Conceptualization, Formal analysis, Methodology, Writing - original draft, Writing - review & editing. Monica Riva: Conceptualization, Formal analysis, Methodology, Writing - original draft, Writing - review & editing, Supervision, Funding acquisition. Alberto Guadagnini: Conceptualization, Formal analysis, Methodology, Writing - original draft, Writing - review & editing, Supervision, Funding acquisition.

**Declaration of interests**

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

The authors declare the following financial interests/personal relationships which may be considered as potential competing interests: