Author response on "egusphere-2022-81"

3D hydrogeological parametrization using sparse piezometric data

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Dear Referee, the additions/modifications are highlighted in yellow in the track-changes version of the manuscript uploaded in Egusphere. We list below the changes corresponding to each of your remarks.

Dear authors I believe your manuscripts is a useful input but reading it I have the following concerns for clarifications and potential improvements.

We thank you greatly for your remarks and your input that really benefited our work.

The interpolation and geostatistical part needs improvement in terms of variogram calculation, stationary analysis, parameters calculation, validation and variance-uncertainty. It is a major part of your methodology and needs to be clear. You mention application of universal cokriging, of which variables, using which variogram model e.t.c

GemPy performs a cokriging of two types of data: isosurface (i.e. the interface between stacked lithologies) and the interface orientation. It uses an arbitrary spherical covariance function that only balances the relative weight of the surfaces and their orientation in the cokriging, as the random function defined in GemPy's method does not bear any physical meaning and is dimensionless. It only aims at ensuring equality at every point of the isosurface.

We propose to add the following information to this section [in brackets, the text was already in the previous version of the manuscript]:

[As a result, the cross-variogram, inherent to cokriging, cannot be empirically determined. The shape of the surfaces mainly depends on the orientations provided and on an arbitrary spherical covariance function that only balances the relative weight of the surfaces and their orientation in the cokriging.] Hence, the variogram parameters do not bear any physical meaning as well and are arbitrarily chosen to ensure stability to the computation according to the GemPy's developers' guidelines (De la Varga et al., 2019): the nugget effect should be small (set to 10 in our case) and the range equal to the domain's extension (10,000 m in our case). As the variogram is not differentiated according to the search direction, the vertical component of the model must be exaggerated (x500 in our case) so that its dimension is compatible with the previously quoted values.

Finally, GemPy produces a 3D facies model made of 50 x 50 x 10 hexahedron elements. After rescaling on the z-direction, it has the same extension as the mesh used for the other models and a finer resolution. Henceforth, the facies in the flow/transport mesh for TRACES are determined according to the majority facies of the GemPy elements intersecting each 3D prismatic element.

it seems that an uncertainty analysis has been carried out in line 280 but it is not clearly presented and discussed. As long as simulations have been carried out then the overall uncertainty can be presented in the facies of the models as support figures.

The uncertainty attached to the optimization step is now introduced in the methodology:

The objective function of the optimization problem takes the form of Eq. 7.

$$O = \sum_i \left(\left(\sum_j l_{i,j} p_j - P_i \right)^T \boldsymbol{\sigma}_i^{-1} \left(\sum_j l_{i,j} p_j - P_i \right) \right) \quad (7)$$

where O is the objective function, i is the index for the constraint (i.e. the sampled location retained for the optimization), j is the index for each facies and $l_{i,j}$ is the thickness [m] of facies j at location i. p represents the parameters to be optimized (the hydraulic conductivity or the effective porosity of each facies) and P the 2D mean values calibrated during the inversion stage, weighted by the matrix $\boldsymbol{\sigma}$ representing this calibration uncertainty. We consider only the diagonal of the matrix, containing the inverse of the variance given at location i by the 2D calibration.

The final uncertainty of the optimized parameters is given by Eq. 8.

$$\epsilon_p = \varphi \left(\frac{\hat{O}}{m} \right)^{1/2} \left(\boldsymbol{C}_p \right)^{1/2} \quad (8)$$

where ϵ_p is the uncertainty of the parameter p, $\hat{O}$ is the objective function at end of the optimization and m is the number of data. The coefficient φ is determined through a Fisher's distribution, assuming a normal distribution of the uncertainty (for an estimation at 95 % of confidence, φ = 1,96). $\boldsymbol{C}_p$ is the variance of the parameter p, derived from the Jacobian (sensitivity matrix) of the model.

The integration of the variance of the 2D parameters slightly modifies the 3D optimized values and allows to give confidence intervals on the final facies parameters (see Sections 3.3 and following).

Your method needs to be compared with a classical 3d inverse modelling approach (3D inverse modelling of groundwater) such the ones that have been published by J. J. Gómez-Hernández and Kitanidis.

The work of J. J. Gómez-Hernández and Kitanidis is added in the introduction, along with the work of Straface and Guadagnini, to better stress the difference with classical 3D inverse modelling approach, that still rely on more heavy and specific data collection:

[But the latter is less sensitive to the vertical structure of the aquifer, leaving its estimation dependent on complex and expensive field methods – e.g. pumping tests (De Caro et al., 2020), tracer tests (Linde et al., 2006), electrical resistivity (Coscia et al., 2011; Priyanka & Mohan Kumar, 2019), radar tomography (Boni et al., 2020), self-potential methods (Eppelbaum, 2021), crosshole testing (Klotzsche et al., 2013; Doetsch et al., 2010), hydraulic tomography (Sanchez-León et al., 2015; Luo et al., 2020; Fischer et al., 2020) – and/or laboratory analysis – e.g. grain-size analysis from core samples (Marini et al., 2018) and ex-situ permeability tests (Zhang & Brusseau, 2005).] The collection of these information, describing the vertical heterogeneity of the aquifer, allows the development of 3D inversion techniques. For example, some successful methods combine direct parameter quantification and stochastic geological modelling (Guadagnini et al., 2004; Fu & Gómez-Hernández, 2008; Cardiff & Kitanidis, 2009), others incorporate water head data and more advanced geophysical measurements to the (joint) inversion procedure (Straface et al., 2011; Lee & Kitanidis, 2014).

In the abstract it is mentioned: Finally, the parameters of each facies (hydraulic conductivity and porosity) are obtained through an optimization loop, that minimizes the difference between the 2D calibrated transmissivity and the transmissivity computed with the estimated 3D facies parameters.

According to presented methodology to achieve the target inversion, interpolation, optimization is applied. All these steps consider parameters. Therefore, an uncertainty analysis is required to study the uncertainty propagation even for synthetic data or at least show the overall uncertainty thorough the simulations, or even identify the sources of uncertainty for the readers to consider them when up-scaling.

Uncertainties concerning the 2D inversion (i.e. the dispersion of transmissivities amongst the different solutions) is now propagated to the optimization (i.e. uncertainty of the facies parameters).

Uncertainties concerning the interpolation has been circumvented by integrating in the parameter optimization only location where the lithology is known.

In addition, the uncertainty occurring when classifying the facies is mentioned but not addressed in this paper. As well, transport parameters are not estimated, as stated in the conclusion, it should be the subject of further research.

Also, a note has been added to make the reader aware of the existence of uncertainty in the water head data (in Section 2.2.):

Although piezometric data is subject to uncertainty in a field context, we do not address this aspect in the present study and the water heads measurements errors are considered as negligible.

The need of comprehensive uncertainty and sensitivity analyses is outlined in the conclusion.

for the B-splines method you mention that one can use GIS, for interpolation python and for the model fortan!
How all these software results are connected for your complete model? It seems that many assumptions should be made and I am still worried about uncertainty.

More information about the bridges between the different tools is added. Concerning GemPy, see above (response to the first comment).

Concerning the GIS procedure for B-spline:

[To avoid anomalies in the stacking of the facies, the interpolation is carried on their thickness instead of their boundaries' z-coordinates. In addition, the first underlying facies is not interpolated but considered as the background (filling) lithology.] The thicknesses of the four remaining facies are delivered in raster format, with integer values between 0 and 10 (i.e. the number of layers in the final 3D model), and a resolution of 200 m. Eventually, the facies stacking is transcribed for each column of prismatic elements in the 3D flow/transport mesh for TRACES according to the same majority analysis as for the GemPy procedure.

TRACES and PINOGRI share the same code language and the same mesh structure (apart from the vertical dimension).

The figures caption require more complete descriptions.

More information has been provided in each figure's caption.

in 3,2: Differences in the facies composition of the models are marginal. ok but are they correct/reliable to be incorporated in the model?

The purpose of the flow/transport simulations is to verify whether the level of error produced by the interpolations (combined with the optimization error on the facies parameters) is compatible with the use of the method for practical purposes (reproduction of piezometric records and pollution plumes).

How the maximal discrepancy is 61 % of the initial value for the permeability and other increased discrepancies mentioned interprets a successful reconstruction of the aquifer dynamics. Obviously the model parameterization works well. Please explain clearly.

Compared to the previous version of the article, the optimization step has been changed in two ways:

The lithological constraints for the 3D optimization being only taken on location where the log is available, the potential interpolation errors are not reported anymore at this stage. Therefore, the optimization produces only one set of facies parameter per sampling (in this case, this step became independent from the lithology interpolation).

The optimization now integrates the 2D parameter uncertainty.

With this new setup, the maximal discrepancy (only considering the optimized value, and not its interval of confidence) is 45.5 % of the initial value, in a linear scale (namely 6.8x10-4 m/s vs 1.25x10-3x10 m/s). In addition, the confidence interval intersects the reference value (see Fig. 6 in Section 3.3). This kind of discrepancy is a small gap in the field of hydrogeology and at our scale of study. The illustrations with the piezometric series (and to a lesser extent the transport results) confirm it.

In figure 7 there are several dashed lines color, please elaborate. In addition, the aim of the work is a 3d hydrogeological characterization combining inversion, interpolation and optimization. It is not clear what fig 7 adds to the work and interpolation techniques application to water level. From the method and flowchart it seems that the interpolation applies to lithological data only.

To make the results figures more readable, now only the sparse sampling outputs are reported, with their confidence intervals (dotted and dashed envelope curves). These confidence intervals are produced by the extreme values amongst 4 supplementary simulations where the parameter values are set: (i) at the upper bound of the confidence interval, (ii) at the lower bound, (iii) alternately at the lower (for the facies 1,3,5) and upper (facies 2,4) bounds, (iv) alternately at the lower (for the facies 2,4) and upper (facies 1,3,5) bounds of the parameter confidence interval.

The water heads and contamination data are here to validate the methodology, i.e. to assess its ability to reproduce state variable of interest in the field of hydrogeology.

The level of consistency between the piezometric chronicles in particular attests that the discrepancies produced beforehand (during facies interpolation and parameter optimization) are marginal or acceptable at least.

line 400: Comparatively to joint inversion methods, the need of data acquisition and the computation efforts are lower. I do not fully agree, here you have uncertainty that you have not discussed. Stating this you need to support it with an example or literature.

The difference between our method and joint inversion in terms of data acquisition is stated in the introduction. There is no classical 3D approach that can rely on piezometric series only, without the help of direct measurement or geophysical surveys. Moreover, computation and even more inversion of 3D models is costlier in CPU than 2D models (with an otherwise equal level of refining on the horizontal dimensions).

reproduction of this work by the readers is not clear, please show some guidelines.

The first part of “Materials and methods” sums up the methodology. To reproduce it, one has to (i) estimate transmissivity from a 2D calibrated flow model, (ii) interpolate borehole data to obtain a 3D facies model, (iii) estimate the individual facies parameter through an optimization algorithm comparing the 2D transmissivity from (i) and the 3D transmissivity resulting from the optimized values.

The model results seems good in the analysis but a sensitivity analysis and uncertainty analysis in my personal opinion is needed to support the findings.

Uncertainties concerning the 2D inversion (i.e. the dispersion of transmissivities amongst the different solutions) and the optimization (i.e. 95 % interval of confidence for the facies parameters) are provided.

A more comprehensive uncertainty propagation and a sensitivity analysis will be performed on a following work.