ADDING GEOLOGY TO THE EQUATION: TOWARDS INTEGRATING STRUCTURAL GEOLOGICAL DATA INTO INVERSE MODELING WITH iTOUGH2

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ABSTRACT

The subsurface structural setting, as a part of the conceptual model, can have a strong influence on the outcome of a flow simulation. The structural geological model should therefore be considered in uncertainty studies or parameter estimations. However, in practice, this inclusion is not easily possible, because the generation of an input mesh for a flow simulation, populated with properties according to a geological model, requires at least some manual work. We present here a method that removes this gap between geological data and flow simulation and propose that it will enable insights into the significance of structural uncertainties in the context of inversion modeling that is not yet possible.

Practical applications of the methods are demonstrated with two simple examples: the inversion of the distance to an impermeable boundary in an aquifer, and the significance of uncertainties in the exact position of structural geological observations, in a CO_2 injection scenario with possible leakage over a fault with an uncertain position.

The presented examples show that the integration of geological structures into an inversion framework enables a consideration of structural uncertainties that is not easily possible with the methods available to date. Geological data can be highly uncertain and limited, and our examples emphasize the fact that these uncertainties can strongly influence the outcomes of a flow simulation.

INTRODUCTION

Structural representations of the subsurface, commonly called geological models, are an important part of the conceptual model and therefore a relevant part of most realistic large-scale flow simulations (e.g., Bundschuh and Arriaga, 2010). It is well known that these geological models contain uncertainties for a variety of reasons, and several recent developments address the analysis of these uncertainties (Thore et al., 2002; Turner, 2006; Wellmann et al., 2010; Lindsay et al., 2012). Furthermore, recent studies show that these uncertainties in the geological model can have a significant influence on flow simulations that are based on these models (Nilsson et al., 2007; Refsgaard et al., 2012).

Even though it is widely accepted that geological uncertainties should be considered in flow simulation studies, this is usually not done in most practical applications. An important reason for this neglect is the lack of an integrated workflow that combines all relevant steps, from the initial structural geological data, to the flow simulation and result analysis, into a coherent inversion framework. We propose here a method to overcome this limitation with a completely automated workflow that combines novel geological modeling methods with TOUGH2 flow simulations in an inversion framework with iTOUGH2. As a test of feasibility, we apply the workflow to test the integration of geological data in flow inversion and uncertainty propagation studies, using two synthetic examples.

MATERIALS AND METHODS

Our aim is to combine geological modeling with the multiphase flow simulation code TOUGH2 (Pruess et al., 2011). We apply here a method that combines and automates TOUGH2 preprocessing methods with the inverse and parameter estimation package iTOUGH2. Specifically, we use a recently developed Python module library that efficiently wraps TOUGH2 input files and greatly simplifies the mesh generation (Croucher, 2012). This library is combined with the inverse capabilities of iTOUGH2, making use of the PEST interface

(Finsterle and Zhang, 2011). Furthermore, we combine these methods with an innovative geological modeling approach based on an implicit potential-field method (Lajaunie et al., 1997) to allow the consideration of complex geological structures in the workflow. The most relevant aspects of the workflow are described in the following.

An overview of the workflow is presented in Fig. 1. The method is centered around iTOUGH2. iTOUGH2 itself was developed as a sensitivity analysis, parameter estimation, and uncertainty propagation package for TOUGH2 simulations (Finsterle, 1999). An iTOUGH2 run commonly incorporates the definition of uncertainties for specific input parameters, the forward simulation for a given problem with TOUGH2 for these parameters, and then the output analysis and comparison to actual observations (see Fig. 1 bottom right). For different types of analyses, these steps are repeated a certain number of times, for example to determine an optimal input parameter set, or to test how uncertainties in the input parameters propagate to flow field observations (e.g. Finsterle, 1999).

The capabilities of iTOUGH2 are accessible for other pre- and post-processing methods through an interface defined with template and instruction files (Finsterle and Zhang, 2011). Interface types are based on the widely used parameter estimation package PEST (Doherty, 1994); template files can be used to control parameters with iTOUGH2 that are not parameters of a TOUGH2 simulation itself (see Fig. 1 bottom left). In addition, the PEST interface can be used to include simulation results from external simulations into the iTOUGH2 framework using instruction files. For more details on the interface and its possibilities, see Finsterle and Zhang (2011).

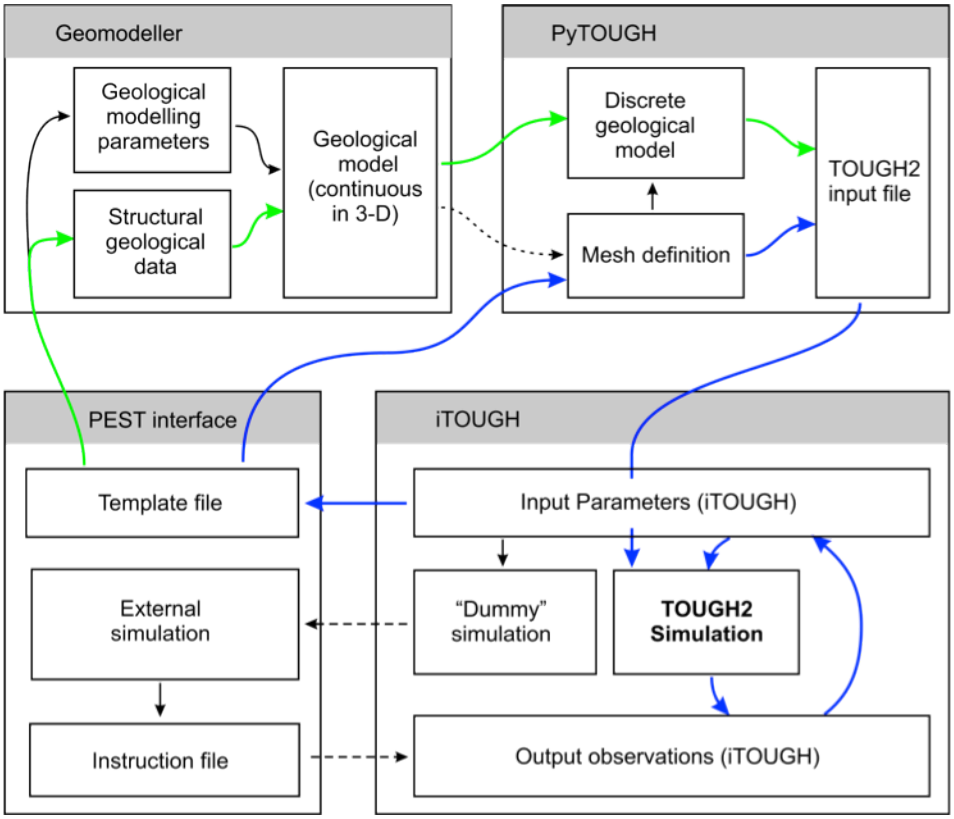

Figure 1. Workflow for the combination of structural geological model construction with iTOUGH2 inversion and model calibration methods

We combine the functionalities of iTOUGH2 here with two external modules: the TOUGH2 preprocessing methods of the Python library PyTOUGH (Croucher, 2012; Wellmann et al., 2011), and the geological modeling methods of a commercial geological modeling package, GeoModeller (Calcagno et al., 2008).

PyTOUGH is a set of modules designed to simplify the input file generation for TOUGH2 simulations, and to provide powerful data analysis and visualization methods (Wellmann et al., 2011). It is written in Python, an open-source interpretative programming language that provides powerful numeric and scientific methods, and data visualization techniques (e.g., Langtangen, 2008). Both PyTOUGH and Python are available at no cost.

We are using here the functionality of PyTOUGH to generate input meshes and input files for TOUGH2 simulations that can be adapted to several structural parameters and considerations (Fig. 1 upper right). The libraries provide several convenient ways that greatly simplify the generation of mesh structures.

We extended the functionality of PyTOUGH with an interface to an innovative geological modeling method (Fig. 1, upper left), implemented in the commercial geological modeling package Geomodeller (www.geomodeller.com). The geological model is constructed through an implicit potential-field interpolation method (Lajaunie et al., 1997). This method enables the interpolation of a full 3-D geological model directly from geological data, implicitly respecting realistic geological constraints (Calcagno et al., 2008). The advantages of this method over standard surface interpolation approaches (e.g., Caumon et al., 2009) are that it enables the automatic reconstruction of a model when the geological input data are changed, and that it is possible to construct realistic 3-D models with a relatively small input data set (e.g., Maxelon and Mancktelow, 2005; Putz et al., 2006; Joly et al., 2008; Calcagno et al., 2012). We consider both aspects as essential for the consideration of structural geological modeling in an inverse simulation context.

The developed workflow can be used in a variety of ways to include different types of pre-processing methods into the inversion frameworks of iTOUGH2. We will use it here along two lines: the automation of mesh and input file generation (indicated by blue arrows in Fig. 1), and the additional combination with the geological modeling module (highlighted with green arrows in Fig. 1). In both scenarios, we will evaluate how the developed workflow enables insight into the relevance of structural geological model uncertainties in the context of flow simulations, and how these uncertainties can be considered.

APPLICATION

Example 1: Inversion for the distance to an impermeable boundary

Pressure drawdown curves, determined during pumping tests in an aquifer, contain important information about hydrogeological properties and the general structure of an aquifer (e.g., Marsily, 1986). It is well known from theory that an impermeable boundary in the vicinity of a pumping well has an influence on the pressure drawdown curves, and analytical methods exist

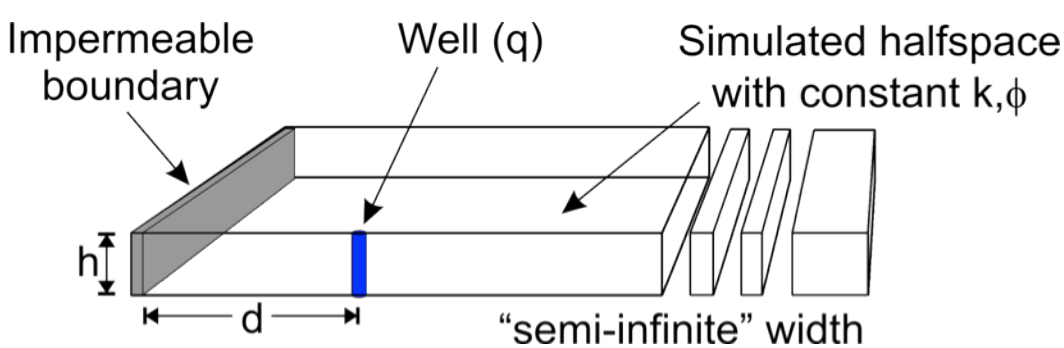

Figure 2. Conceptual model set-up for the pumping half-space model: the simulation is performed in a semi-infinite half-space with an impermeable boundary in an unknown distance d to the well. Additionally, aquifer thickness h and permeability k are considered uncertain.

Table 1. Initial parameters and results determined in different inversion scenarios; results are given with the estimated marginal standard deviation apart from the case of perfect data, where it is negligible.

Parameter	Correct value	Initial Guess	Perfect Data	Noise "1"	Noise "2"	Thickness and Noise
log10(k) [k in m^2]	-12	-11.5	-12	-12 + 0.005	-11.9 + 0.04	-11.9 + 0.026
d [m]	40	100	40	42 + 3.62	34 + 24	36.4 + 3.11
h [m]	20	(25)	(fixed)	(fixed)	(fixed)	17 + 7.84

to determine this influence (Ferris et al., 1962).

In this first example, we apply the developed workflow as a simple method to determine the distance to an impermeable boundary from observed (and potentially noisy) pressure drawdown data.

Model setup

We consider here a simple hydrogeologic setting of a confined aquifer with constant thickness, with an impermeable boundary at one side and a quasi-infinite extension in all other directions. The conceptual model is shown in Fig. 2: the well is placed in a distance d to an impermeable boundary. The aquifer is semi-infinite, with constant permeability k and porosity ϕ, and of constant thickness h. Pumping is performed for two days with a constant rate q.

We use here the part of the workflow that enables an automatic mesh generation and TOUGH2 input file generation with PyTOUGH, with the inversion framework of iTOUGH2, as highlighted by the blue arrows in Fig. 1. The only structural ("geological") input parameter in this case is the distance d to the impermeable boundary. The parameter is updated in every iTOUGH2 iteration, then passed through the PEST interface to adapt a template file that is then used to generate an adapted mesh, before the next TOUGH2 simulation. Two map views for generated meshes with a distance of 30 m, and a distance of 60 m between well and impermeable boundary are shown in Fig. 3, with the simulated pressure distribution in the aquifer after two days of pumping, highlighting the obvious effect of the boundary on the pressure distribution.

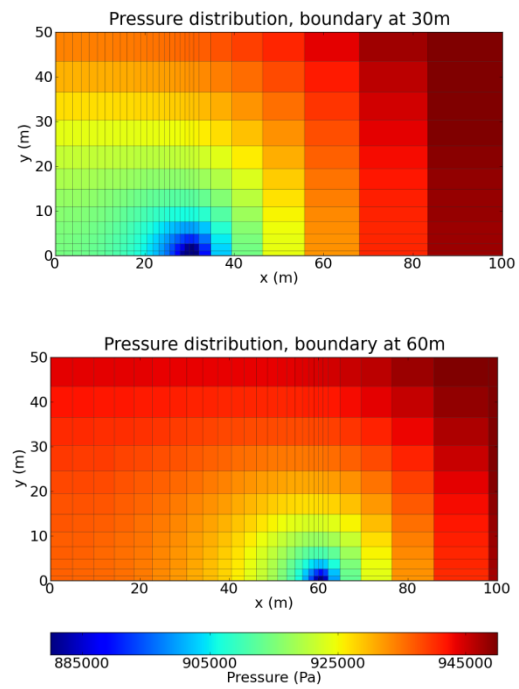

Figure 3. 2-D Map view of pressure distribution in the aquifer after two days of pumping for two different distances between impermeable boundary and pumping well: the different pressure distribution around the well is clearly visible.

An initial synthetic pressure drawdown curve for the following inversion studies is determined for the parameter settings d = 40 m, h = 20 m and k = 1E-12 m^2 (Tab. 1). A total of 192 measurements are simulated over the pumping period of two days (blue curve in Fig. 4). We will now apply the workflow to invert for the aquifer permeability and the distance to the impermeable boundary in several scenarios.

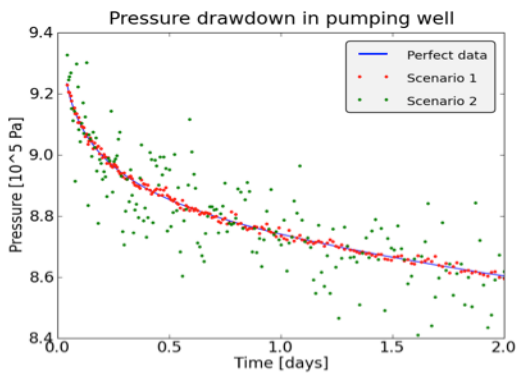

Figure 4. Pressure drawdown curves: initial synthetic drawdown curve (blue line) and measurement scenarios with added random noise (red dots: low noise, green dots: high noise)

Inversion results

In a first step, we test the workflow for a joint inversion for aquifer permeability and the distance to the impermeable boundary for a perfect data set, i.e. we take the generated synthetic pressure drawdown curve as observed data. As a first guess, we assume that we considered the permeability as a bit too high (k = 5E–11 m^2) and that there is no impermeable boundary in the close vicinity of the well (d = 100 m). In this case, the method determines both the position of the impermeable boundary and the aquifer permeability perfectly well (Tab. 1 "Perfect data").

With some more simple tests, we now evaluated how the inversion performs in the case of noisy data. We generated two data sets with added random noise to the observations to simulate measurement error. In the first scenario, we added small random Gaussian error with a standard deviation of σ = 1000 Pa, and in the second case a higher error with σ = 10,000 Pa.

For both scenarios, the aquifer permeability is determined almost perfectly (Tab. 1). The distance d to the impermeable boundary is overestimated by 2 m in the case of low noise, and underestimated by 6 m in the case of high noise, although the estimated standard deviation is very high.

As a further comparison of the behavior of the objective function in the case of the high-noise scenario, a grid search was performed over a range of 30–50 m for the distance d, and -12.25 to -11.75 for $\log_{10}(k)$ for the logarithm of permeability (Fig. 5). The grid search results show that permeability in this range can be well determined in both cases, a behavior that is reflected in the results presented in Table 1. The distance to the impermeable boundary is more difficult to estimate with high accuracy, and the determination is only very vague in the case of the highly noisy data (Fig. 5b).

In the third scenario, the performance of the inversion scenario is evaluated for an additional uncertain structural geological parameter: the thickness h of the aquifer. The inversion is performed for an initially overestimated aquifer thickness of 25 m. The inversion performed well in determining the permeability and reasonably well in determining the distance to the boundary (although the real value is outside of one standard deviation σ). In this case, the aquifer thickness is not very well determined with the amount of observed data.

<u>Example 2: CO2 injection and potential leakage over</u>

In the second example, we apply the entire workflow, including geological modeling (upper left in Fig. 1, combined along green arrows), to evaluate the sensitivity of a flow simulation directly with respect to structural geological observations in a more complex scenario. The flow simulation considered here is a synthetic example of simulated CO_2 sequestration into an anticlinal structure, with potential leakage over a fault in the vicinity (Fig. 6a).

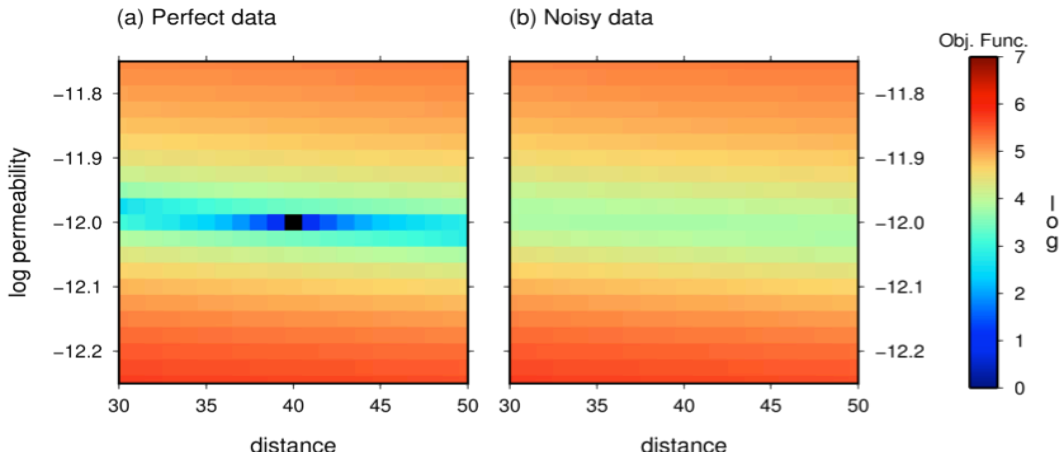

Figure 5. Results for grid search of objective function for the case of (a) perfect data, and (b) a noisy dataset (second scenario with high noise, green dots in Fig.); The grid search results suggest that it is in both cases possible to invert for the permeability, but the determination of the structural uncertainty, the distance to the impermeable boundary, is problematic for high noise.

Model setup

The geological modeling method that we implemented in the workflow is capable of representing complex 3-D geological structures with relatively few input parameters. We use it here to construct a 3-D model of a folded sedimentary pile that is intercepted by a fault (Fig. 6a). The sedimentary pile comprises three layers and is folded, with an anticlinal structure in the center of the model. The sedimentary pile (including the folding) is parameterized by four geological surface contact points ("control points" in Fig. 6a) and the fault by three points. As further geological constraint, the sedimentary layers are defined to be subparallel and offset by the fault (see Calcagno et al., 2008, for more details about geological logic and implementation). With these geological settings, and additional interpolation parameters, the seven contact points are sufficient to describe the entire geological model in full 3-D (Fig. 6b).

The geological model is a continuous representation in 3-D. To use it as a conceptual model for a TOUGH2 simulation, it needs to be discretized. As before, we use PyTOUGH for the mesh generation (Fig. 1). We create here a simple regular mesh with a defined number of elements in each coordinate direction. An extension module for PyTOUGH is then used to determine the size of the geological model to set up the mesh structure. In a next step, for each cell in the mesh, the geological unit (i.e., the "rocktype") is determined from the geological model; in this way, the continuous geological model is mapped onto the discrete mesh structure (Fig. 6c). The mesh information is then combined with a template TOUGH2 input file that contains definitions for rocktypes, the CO_2 source, and other model settings.

The CO_2 injection and subsurface flow are simulated with the TOUGH2 fluid property module for mixtures of water, NaCl, and CO_2: ECO2N (Pruess and Spycher, 2007). Rocktype, source, and modeling parameters are adapted from the second example in the manual (Pruess, 2005), the (radial) flow from a CO_2 injection well (rcc3). We use here the same basic settings, i.e., injection into a reservoir with constant temperature, consideration of salt precipitation without associated permeability reduction. Initial pressure is 120 bar.

The properties of the rock types for the different geological units are adapted from the "sand" and "shale" rocktypes of "Problem No. 4 (rtp7)" of the ECO2N manual (Pruess, 2005). The "shale" properties are assigned to the reservoir cap (see Fig. 6b), and "sand" properties to all other geological units. The permeability of the cap is set to k = 1E-18 m^2 and to 1E-12 m^2 for the other units.

Sensitivity study

An important consideration in any CO_2 injection scenario is the possible leakage of CO_2 to the surface, e.g., over a fault in the vicinity of the injection site. It is a common case in the early stage of a feasibility study that the subsurface structural setting is highly uncertain. In the case of the conceptual model considered here (Fig. 6a), uncertainties are considered directly for the surface contact points (indicated with error bars around the contact points in Fig. 6a). We now use the developed framework combining geological modeling with iTOUGH2 to test which data point uncertainties have the highest influence on potential leakage over the fault, with a sensitivity study.

We consider the change of total mass of CO_2 in the undifferentiated geological unit to the West of the fault as indicator for fault leakage. The parameters included in the analysis are the z-position of the surface contacts point defining the reservoir-seal boundary (points R_W and R_top, in Fig. 6a), and the E-W position of the point defining the fault (point F in Fig. 6a). All values are assigned a normal distribution with a standard deviation of 100 m. Additional parameters could be considered, for example the thickness of the seal, but for simplicity we restrict the analysis to these three parameters as a first test.

The results of this analysis are shown in Fig. 7. The total parameter sensitivity is highest for the structural geological contact point that defines the top of the reservoir, R top (see Fig. 6a). In addition, the data point that defines the western side of the reservoir, R_W, is important for the consideration of fault leakage. However, the data point that defines the actual position of the fault, F, is less relevant in this analysis.

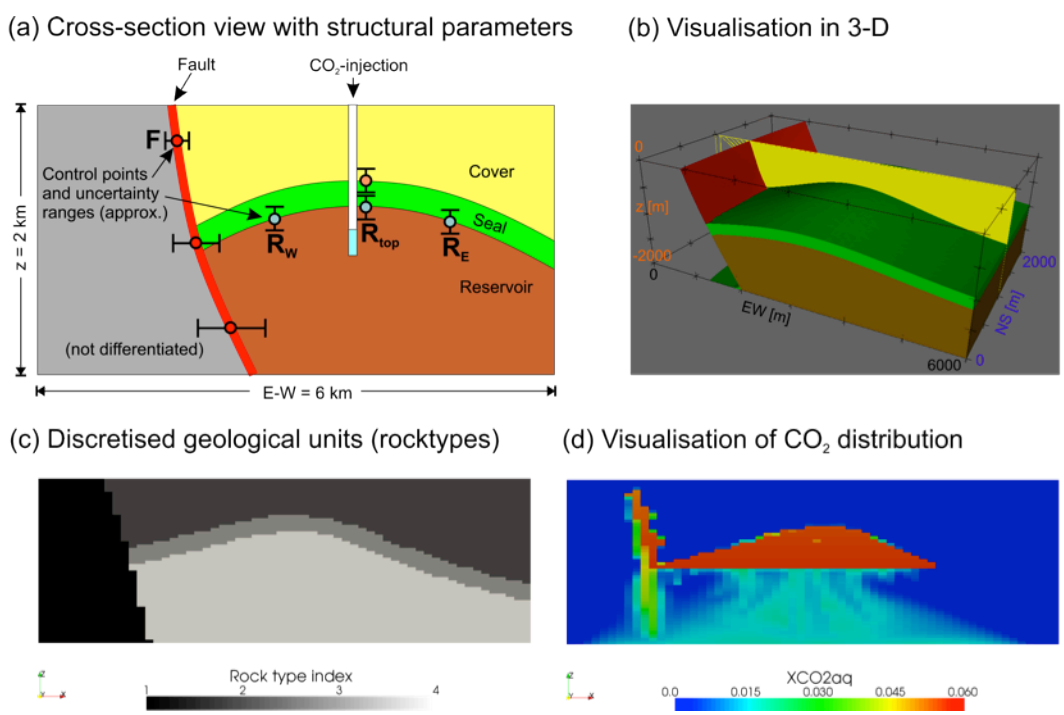

Figure 6. (a) Conceptual model for a CO_2-injection scenario with an uncertain distance to a fault: the figure shows a 2-D section through the model; CO_2 is injected into an anticlinal structure. The points denote contact points between geological units with an uncertain position; (b) full 3-D view of the model; (c) discretized model in a 2-D slice; (d) example of simulated CO_2 distribution with leakage over fault

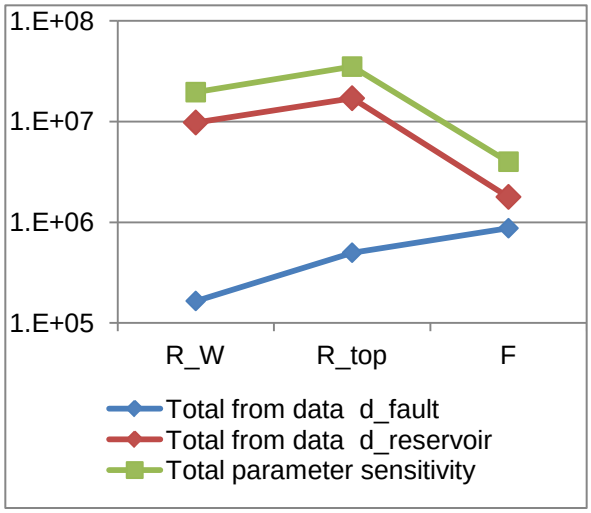

Figure 7. Parameter sensitivity for three geological contact points

DISCUSSION

The geological structure is an important aspect of subsurface uncertainties. Here we presented a method to include it in the framework of multiphase flow simulations with TOUGH2. The most important feature of the geological modeling that we integrated here is that it allows the representation of complex and realistic 3-D structural geological settings with a relatively small parameter set. This feature is an important prerequisite to integrating it into an inverse framework.

As a test of feasibility, we applied the workflow to two synthetic examples: in the first case, we used the methods to invert for the distance from a pumping well to an impermeable boundary in an aquifer, using the pressure drawdown in the well.

In the second example, we addressed the more complex problem of combining geological modeling and multiphase flow simulations: we evaluated how uncertainties in the subsurface structure influence fluid flow predictions. We considered a scenario in which CO_2 was injected into an anticlinal structure, with a possible leakage over a fault in the vicinity. Both examples show that it is possible to consider geological information in an inverse flow simulation framework, as an important step forward for adding geological data into uncertainty estimations of flow simulations.

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