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Flexible simulation framework to couple processes in complex 3D models for subsurface utilization assessment

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Abstract

Utilization of the geological subsurface for production and storage of hydrocarbons, chemical energy and heat as well as for waste disposal requires the quantification and mitigation of environmental impacts as well as the improvement of georesources utilization in terms of efficiency and sustainability. The development of tools for coupled process simulations is essential to tackle these challenges, since reliable assessments are only feasible by integrative numerical computations. We have been developing a flexible numerical simulation framework, providing efficient workflows for integration of data and software packages for coupled process simulations and introduce three case studies to demonstrate its capabilities.

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Keywords: Geological subsurface utilization; Numerical simulation; Coupled simulation workflow; Simulation framework; Complex geological models; Hydromechanical simulation; Hydrochemical simulation

1. Introduction

Utilization of the geological subsurface for production and storage of hydrocarbons, chemical energy and heat as well as for waste disposal requires the quantification and mitigation of environmental impacts as well as the improvement of georesources utilization in terms of efficiency and sustainability. The development of tools for

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coupled process simulations is essential to tackle these challenges, since reliable assessments are only feasible by integrative numerical computations [1]. Coupled processes at reservoir to regional scale determine the behavior of reservoirs, faults and caprocks, generally demanding for complex 3D geological models to be considered besides available monitoring and experimenting data in coupled numerical simulations. We have been developing a flexible numerical simulation framework that provides efficient workflows for integrating the required data and software packages to carry out coupled process simulations considering, e.g., multiphase fluid flow, geomechanics, geochemistry and heat. Simulation results are stored in structured data formats to allow for an integrated 3D visualization and result interpretation as well as data archiving and its provision to collaborators.

The main benefits in using the flexible simulation framework are the integration of geological and grid data from any third party software package as well as data export to generic 3D visualization tools and archiving formats. Coupling of the required process simulators in time and space is feasible, while different spatial dimensions in the coupled simulations can be integrated, e.g., 0D batch with 3D dynamic simulations. User interaction is established via high-level programming languages, while computational efficiency is achieved by using low-level languages. In the following, we present three case studies on the assessment of geological subsurface utilization, based on different process coupling approaches and numerical simulations, realized with the help of our simulation framework.

2. From static geological models to coupled simulations and result visualization

Figure 1 shows the general structure of the flexible simulation framework. Proven software packages for geological modelling, numerical simulation and 3D visualization are integrated by the framework, using specific interfaces and coupling modules. This allows us to integrate data from basically any geological modelling software package and grid generation tool available on the market. Arbitrary numerical simulators can be coupled, e.g., flow with chemical and mechanical simulators or flow and process simulators, etc. Hereby, a coupling between simulations using different grid dimensions is also feasible, i.e., coupling 0D geochemical batch simulations with reservoir simulations.

User interaction is realized by using high-level programming languages, e.g., Python [2], while computational efficiency of the interface modules is achieved by low-level programming languages (C++), considering integration of both languages via the Cython C-extensions [3]. An example workflow for data integration and realization of a coupled hydromechanical simulation, including simulation result analysis is given in Figure 2. The simulation framework is continuously further developed and enhanced by innovative workflows, e.g., [4-5].

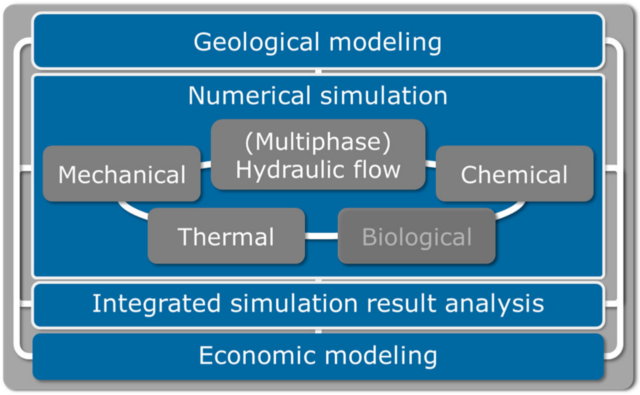

Fig. 1. Flexible simulation framework integrating the full workflow of geological modelling, coupled numerical simulation, result analysis and techno-economic assessments.

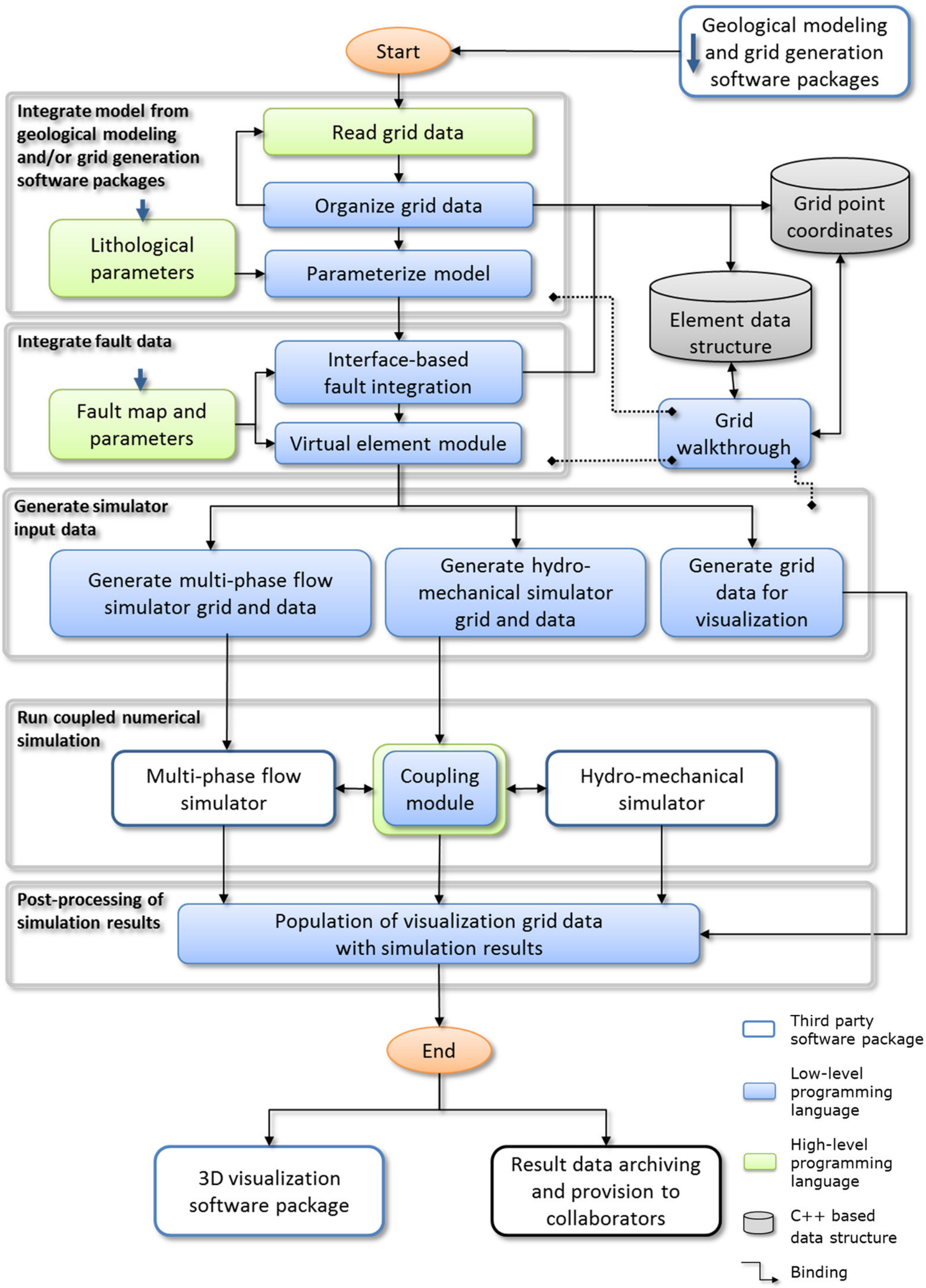

Fig. 2. Flowsheet example for a coupled hydromechanical simulation using the flexible simulation framework.

3. Case studies on geological subsurface utilization assessment

3.1. Coupling hydromechanical simulations to quantify the impacts of enhanced gas recovery

Natural gas from deposits in the Fore-Sudetic Monocline of the Southern Permian Basin has been produced since the early 1970s, inducing significant pore pressure changes in the respective reservoirs. We investigated a prospective enhanced gas recovery operation at the Załęcze gas field by coupled hydromechanical simulations to account for the mechanical integrity of the reservoir, caprock and regional faults (Figure 3). The applied simulation strategy, based on the integration of dynamic flow simulations with hydromechanical ones was carried out using the flexible simulation framework.

Our results indicate that fault reactivation, generating potential leakage pathways from the reservoir to shallower units is highly unlikely due to the low fault slip tendency (close to zero) in the Zechstein caprocks (Figure 4). Consequently, our simulation results emphasize that the supra- and subsaliniferous fault systems at the Załęcze gas field are independent and very likely not hydraulically interconnected [6]. Further successful application examples for coupling hydromechanical processes by means of the flexible simulation framework are given by in [7-16].

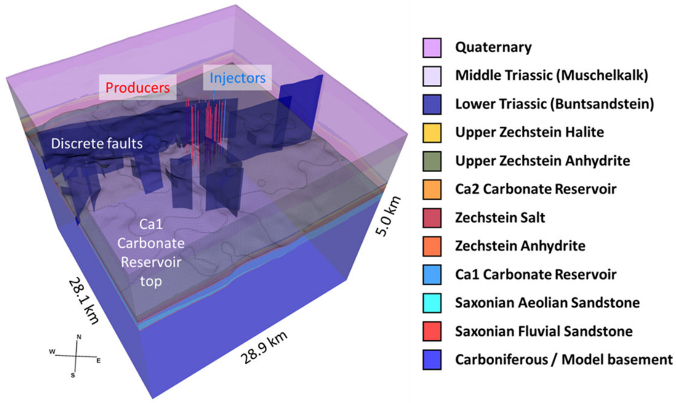

Fig. 3. Lithological units integrated into a regional-scale hydromechanical model of a Polish natural gas deposit, including the discrete faults (blue), the reservoir top (internal gridded surface), hydrocarbon gas production wells (red) and two CO_2 injection wells (light blue) [6].

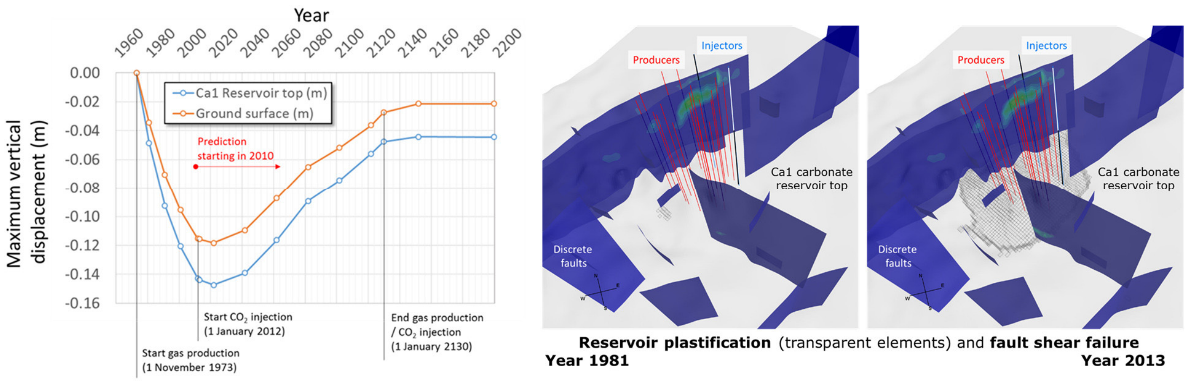

Fig. 4. Calculated maximum vertical displacements (m) at the reservoir top and ground surface during natural gas production (1973-2130) and CO_2 injection (2012-2130) (left). Fault shear failure (non-blue colours at fault planes) as well as plastification in the reservoir (right). Transparent grey layer is the reservoir top. Horizontal distance between the two injection wells (blue) is 1.6 km [6].

3.2. Coupled hydrochemical simulations to quantify CO_2 mineralization and trapping mechanisms at reservoir scale

Long-term integrated site behavior assessment with high spatial resolution on the reservoir scale requires a sophisticated workflow to represent the relevant processes. In our hydrochemical coupling concept, we consider the time-dependent occurrence and significance of multi-phase flow and geochemical reactions. Numerical simulations for the pilot site Ketzin demonstrate that after 10,000 years CO_2 dissolution is the dominating trapping mechanism and mineralization occurs on the order of 10 % to 25 % (Figure 5) with negligible changes to porosity and permeability [12,17-18]. Further application examples of the flexible simulation framework capabilities in coupled hydrochemical simulations and a detailed discussion on integrating 0D geochemical with 3D reservoir models are given in [19-20].

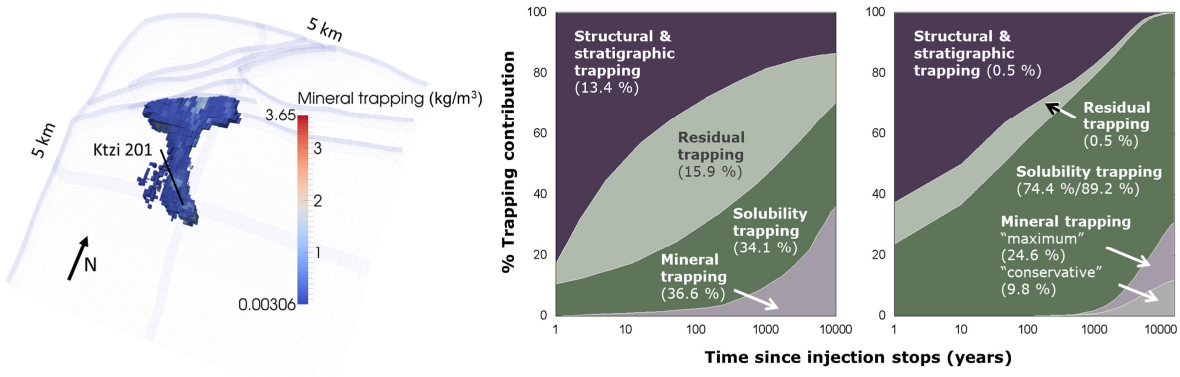

Fig. 5. Carbonate mineralization at the Ketzin pilot site in the Stuttgart Formation after 10.000 years based on coupled hydrochemical simulations (left). Contribution of the four CO_2 trapping mechanisms to increasing storage safety after IPCC [21] (middle) and predicted by coupled numerical simulations for the Ketzin pilot site (right, contribution of each trapping mechanism at 10,000 years is given in the parentheses) [12].

3.3. Coupled thermomechanical simulations to determine permeability changes in the vicinity of an underground coal gasification reactor

Using the flexible simulation framework, we developed a coupled thermo-mechanical model to assess permeability changes in the vicinity of an underground coal gasification (UCG) reactor (Figure 6, left), resulting from excavation and thermo-mechanical effects. Simulation results show that thermo-mechanical rock behavior is mainly driven by the thermal expansion coefficient, thermal conductivity, tensile strength and elastic modulus of the surrounding rock (Figure 6, right). A comparison between temperature-dependent and temperature-independent parameters applied in the simulations indicates notable variations in the distribution of total displacements in the UCG reactor vicinity related to thermal stress, but only negligible differences in permeability changes. Hence, temperature-dependent thermo-mechanical parameters have to be considered in the assessment of near-field UCG impacts only, while far-field models can achieve a higher computational efficiency by using temperature-independent thermo-mechanical parameters (Figure 7). Considering these findings in the large-scale assessment of potential environmental impacts of underground coal gasification, representative coupled simulations based on complex 3D large-scale models become computationally feasible [22-23].

A second application example of the simulation framework in the field of underground coal gasification is given in [24], where we coupled analytical process models with numerical simulations for calculation of conductive heat transport and quantification of the required UCG reactor cool-down time, considering natural heat convection and forced cooling by water flooding. Further, Tillner et al. [25] demonstrate the simulation framework application in synergetic geothermal applications. Examples for the integration of models to assess UCG economics by means of the flexible simulation framework are given in [26-28] and for integration of reservoir simulation with economic analyses in [29-31].

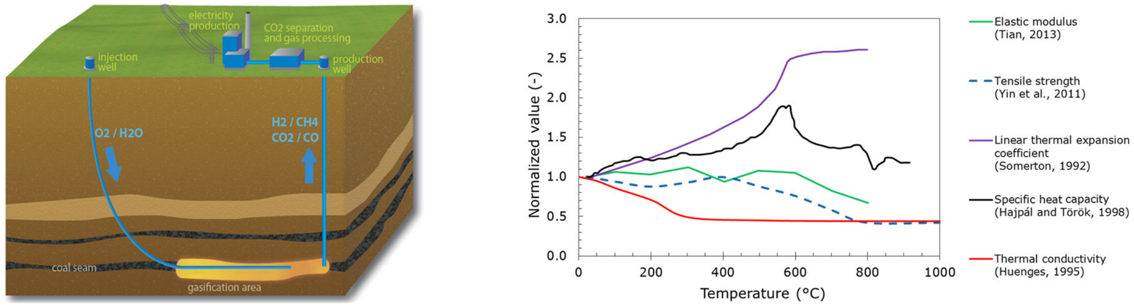

Fig. 6. Conceptual scheme of the combined UCG process [24] (left). Trend of normalized thermomechanical properties of sandstones as a function of temperature [22] (right).

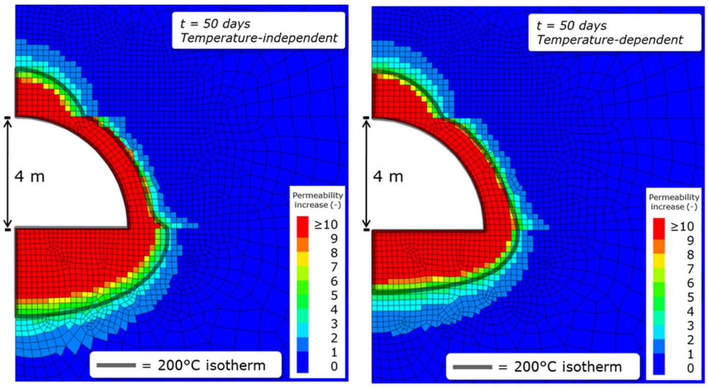

Fig. 7. Temperature- and excavation-induced porosity and permeability changes in the UCG reactor vicinity, expressed as function of volumetric strain increment for temperature-independent (left) and –dependent model parameterizations (right). Grey solid line represents the 200 °C isotherm [22].

4. Conclusions

The development of tools for coupled process simulations is essential to tackle the challenges in geological subsurface utilization, since reliable assessments are only feasible with the support of integrative numerical computations. We have been developing a flexible numerical simulation framework, which provides efficient workflows for integration of data and software packages for coupled process simulations and presented three case studies of geological subsurface utilization, including hydromechanical, hydrochemical and thermomechanical process couplings at near-field to regional scales.

We also briefly discussed and referenced further example studies dealing with large-scale hydromechanical, multiscale hydrochemical and thermomechanical simulation problems in the context of the framework. It has to be noted that arbitrary process simulation tools and mathematical models for economic analyses can be also integrated to establish complex sensitivity analyses. The simulation framework is continuously further developed and enhanced by implementation of innovative workflows and interfaces required to integrate the most powerful geological modelling, simulation and visualization software packages.

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