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Geomechanical integrity verification and mineral trapping quantification for the Ketzin CO_2 storage pilot site by coupled numerical simulations

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Abstract

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 coupling concept we consider the time-dependent occurrence and significance of multi-phase flow, mechanical effects and geochemical reactions. Our numerical simulations for the pilot site Ketzin demonstrate that mechanical reservoir, caprock and fault integrity are maintained during the time of operation and that after 10,000 years CO_2 dissolution is the dominating trapping mechanism and mineralization occurs on the order of 10 % to 25 % with negligible changes to porosity and permeability.

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Keywords: CO_2 storage; Ketzin pilot site; numerical simulations; process coupling; mechanical integrity; mineral trapping

1. Introduction

The Ketzin pilot site located in Germany is the first European on-shore site for CO_2 storage [1-6]. CO_2 injection commenced in June 2008 with about 67,000 tons of CO_2 injected until site abandonment started in August 2013. The Stuttgart Formation (Middle Keuper, Triassic) has an average thickness of about 74 m and is determined by fluvial lithofacies, whereby high-permeable sand channels dominate the multi-phase flow regime in the storage reservoir and provide a net thickness of about 18 m in the vicinity of the injection well (CO2 Ktzi 201/2007, hereafter referred to as “Ktzi 201”) and three observation wells (CO2 Ktzi 200/2007, CO2 Ktzi 202/2007 and CO2 Ktzi 203/2012 [7];

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hereafter referred to as “Ktzi 200”, “Ktzi 202” and “Ktzi 203”, respectively). Recent updates of the geological model, of which general implementation is discussed by Norden and Frykman [8] and Kempka et al. [9], allowed us to revise the so far partially successful history match undertaken by Kempka et al. [10] and now match the simulations with regard to Ktzi 201 and Ktzi 202 bottom hole pressure [11] with very good agreement as well as the arrival times in the observation wells Ktzi 200 (about 50 m distance from Ktzi 201) and Ktzi 202 (about 112 m distance from Ktzi 201) with relatively low deviations [4,12].

Static and dynamic numerical modeling generally accompany the entire CO_2 storage site life cycle. Thereto, it is required to update static and match dynamic models with field observations on a regular basis in order to provide a prognosis on future behavior of CO_2 migration and pressure development as well as to provide an integrated assessment of CO_2 trapping mechanisms. We investigated and predicted the coupled processes at the Ketzin pilot site by numerical simulations using different model coupling schemes. For that purpose, a coupling concept was developed taking into account the time-dependent occurrence and relevance of certain processes involved (thermal, hydraulic, chemical and mechanical) at given time-scales (site operation, abandonment and long-term stabilization phases).

2. Numerical model coupling methodology and workflow

Considering coupled thermal, hydraulic, mechanical and chemical processes in a CO_2 storage reservoir as well as the under- and overburden, numerical models can significantly support the assessment of long-term site behavior. Since static model set-up and dynamic model coupling itself is a highly complex and error-prone process, resulting from e.g. the lack of experimental data indicating the relation between certain parameters, numerical coupling has to be reduced to a level where it is still possible to control it by means of process understanding [13,14]. Given the fact that different processes in the reservoir and surrounding rocks contribute in very diverse ways to long-term stabilization in terms of time dependent relevance (Fig. 1), simplifications of process coupling become a reasonable measure to assess the long-term behavior of a CO_2 storage reservoir. Due to the computational effort a fully coupled model of high spatial resolution covering thousands of years would require, separate analysis of the inherent processes is so far the only way to go.

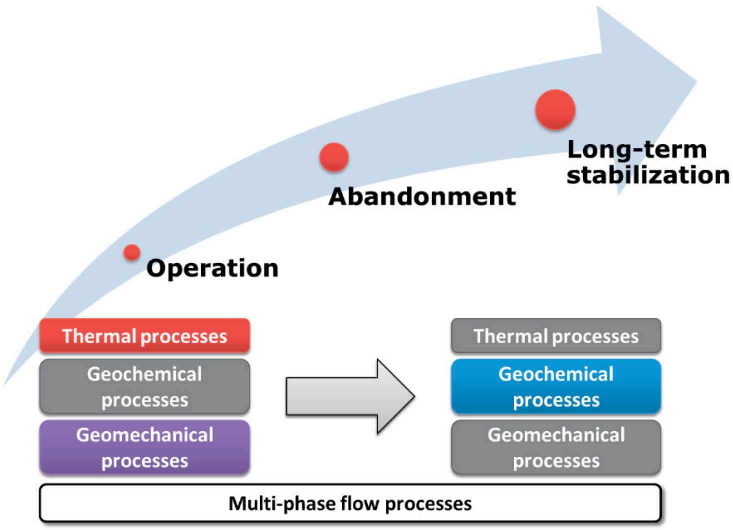

Fig. 1. Time-dependency of processes relevant for site behavior during different life cycle phases of the Ketzin pilot site for CO_2 storage. Besides multi-phase flow, thermal and mechanical processes dominate the operational phase, while geochemical reactions become relevant in the long-term stabilization phase following site abandonment. Grey boxes represent processes negligible in the given phase.

In our coupling approach, we use multi-phase flow simulations as the basis for all other processes, since these represent the observed hydrodynamic site behavior, and also enable us to carry out predictions about long-term site stabilization by means of CO_2 migration and dissolution. Consequently, dynamic reservoir simulations allow for assessment of the structural trapping, residual trapping and solubility trapping mechanisms as discussed in the IPCC report [15] and in Kempka et al. [16] for the Ketzin pilot site.

Thermal processes are only relevant during site operation (CO_2 injection), when the temperature of the injected CO_2 is not equal to the one of the storage formation or CO_2 is migrating into geological units exhibiting a temperature regime different from the initial storage reservoir. At the Ketzin pilot site, CO_2 was heated to formation temperature almost during the entire injection period [17]. Consequently, we neglect any thermal processes in the scope of the reservoir-scale simulation studies conducted for Ketzin.

Depending on the chemical compositions of injected CO_2 and formation fluids present, geochemical processes may be relevant already during site operation. However, considering mineral trapping and long-term stabilization, geochemical reactions have to be taken into account definitely on the long-term (a few hundred years onwards). We have elaborated a simplified coupling scheme between reservoir simulations and geochemical batch simulations [18] that has been validated by De Lucia et al. [19] in order to assess the long-term geochemical fate of the injected CO_2 at the Ketzin pilot site. With that, we are able to underline that geochemical reactions during site operation are of minor importance but play a role regarding long-term mineral trapping in the reservoir.

Geomechanical processes are mainly important during site operation, when significant changes of pore pressure, and thus effective stresses, are encountered. In this context, we carried out hydro-mechanical simulations for the operational period of the Ketzin pilot site indicating that the entire system integrity is not compromised by dynamic pressure changes in the storage formation [20]. Hence, geomechanical processes become only relevant on the long-term, if significant changes due to reactions in the reservoir have to be expected. These may result in changes of mechanical fault properties (e.g. cohesion, friction and dilation coefficients, etc.) due to e.g. dissolution of fault infill minerals. Nevertheless, this behavior is not expected to occur at the Ketzin pilot site, since the current knowledge on mineral composition of the formation and overburden rocks suggest only little changes in porosity as a result of CO_2 exposure [21,22].

In summary, coupled processes are strictly time-dependent and have to be considered using a time-adjusted process model coupling to limit the required computational time and resources in addition to a reduction of error-prone process coupling. Fig. 2 outlines the workflow we follow to study the integrity of CO_2 storage sites in general and Ketzin in particular. Basis is the static geological model serving as input for multi-phase flow simulations with high spatial resolution on and for the required time frame. The results are fed into hydro-mechanical simulations on the one hand and geochemical reactions on the other. In the following, we discuss the final and most considerable part of the process model coupling, the assessment of mechanical integrity as well as long-term mineral trapping at the Ketzin pilot site for CO_2 storage.

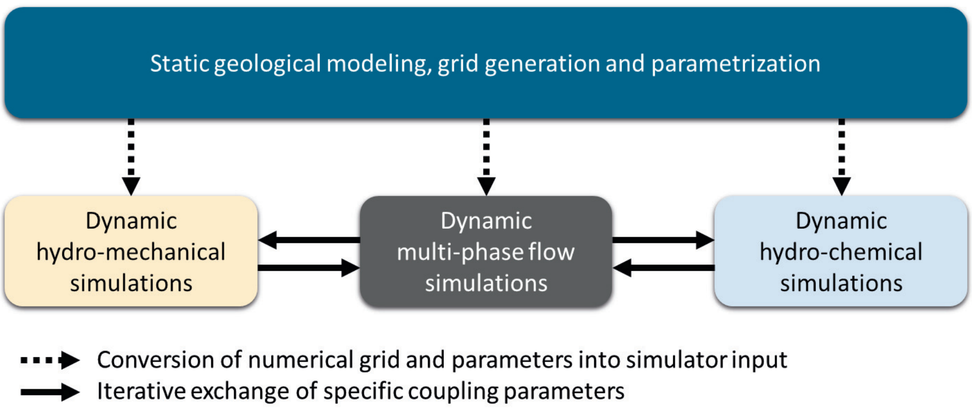

Fig. 2. Numerical modeling and process coupling framework employed for long-term site behavior assessment.

3. Hydro-mechanical integrity assessment

A verification of mechanical integrity of caprocks and faults was undertaken within the scope of a risk assessment prior to the start of injection at the Ketzin pilot site. At that time, only a few data on site behavior as a result of CO_2 injection were available. New data resulting from monitoring, geological model revision [8,9] and from history matched multi-phase flow numerical simulations [10,12] were integrated into our 3D hydro-mechanical numerical simulation models based on a 40 km x 40 km 3D structural geological model taking into account all 24 known major faults in that area. This was then used to determine, if reservoir rock, caprock or fault integrity may be compromised by the CO_2 storage operation carried out [20] using a specific numerical simulation workflow [23].

Maximum vertical displacements at the top of the reservoir (at the Ktzi 201 CO_2 injection well) of about 6 mm and a ground uplift of almost 4 mm are achieved in March 2010 according to our simulation results. Taking into account the ground uplift bowl with a radius of about 3 km, whereas the maximum uplift is concentrated in the close vicinity of the injection wells, an impact in surface structures and installations is not to be expected [20]. Due to the low total amount of CO_2 injected into the storage formation and relatively shallow storage depth at the Ketzin pilot site, the calculated ground uplift in the range of a few millimeters is not directly comparable to those reported from large-scale CO_2 storage projects (e.g. [24-27]) or results obtained from the assessment of prospective CO_2 storage sites (e.g. [28-33]) The latter exhibit induced ground uplift of a few centimeters to decimeters depending on the spatial pore pressure elevation, reservoir depth and radius as well as the mechanical reservoir and caprock properties and fault geometries.

Neither tensile nor shear failure are observed in the coupled hydro-mechanical model at any simulation time step for the rock matrix as well as for the ubiquitous joint elements representing the discrete faults. Regional fault slip tendency is low with a maximum of 0.34 (Fig. 3), whereas fault slip tendency at near-field faults is somewhat lower with about 0.15. Hence, fluid leakage via faults or even fault reactivation as a result of the CO_2 storage operation at the Ketzin pilot site is highly unlikely. Furthermore, in addition to our field observations, the numerical modeling results indicate that integrity of the first caprock above the Stuttgart Formation is not compromised by the pore pressure elevation of about 1.6 MPa. Consequently, we concluded that the mechanical system integrity of the Stuttgart Formation, regional faults and the caprocks is maintained during CO_2 storage operation and in the long-term thereafter [20].

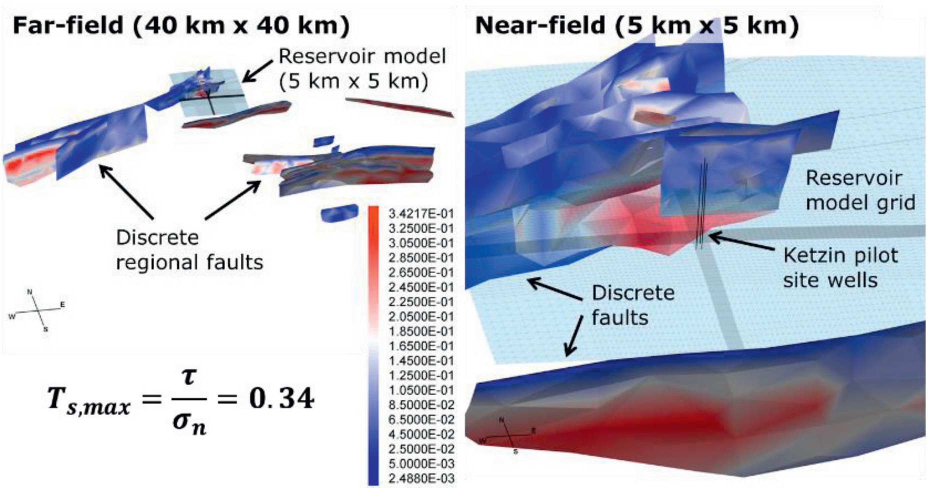

Fig. 3. 3D far-field view of fault dilation tendency of all 24 regional faults. Locations of the Ketzin pilot site wells and multi-phase flow reservoir model are given (left). Close-up 3D near-field view of fault slip tendency. Maximum observed fault slip tendency is $T_{s,max} = 0.34$.

4. Hydro-chemical assessment of long-term mineral trapping

The evaluation of long-term CO_2-induced chemical reactions at the Ketzin pilot site was conducted by means of batch geochemical simulations and coupled reactive transport models as discussed by Klein et al. [18] and Kempka et al. [16]. Reason for that is, as mentioned already above, that fully coupled reactive transport models for long-term simulations at reservoir scale are currently not feasible with the same detailed spatial discretization and same number of grid elements as used in the non-reactive hydrodynamic simulations discussed in detail by Kempka and Kühn [12]. Simulation of reactive transport requires a largely coarsened grid to maintain a low number of elements, which in turn may lead to an oversimplification of the hydrodynamic behavior of a complex CO_2 storage system. To partially overcome this issue, an innovative simplified strategy for the coupling of chemical reactions with multiphase flow, especially suited for long-term CO_2 storage, has been introduced [18]. The distribution of resulting carbonates is presented in Fig. 4. The injected CO_2 migrates along the formation top dip-upward until further migration is hindered by the fault throw at the anticline top, where a graben structure is present. The gas cap structurally trapped at the anticline top is dissolving with time into the formation water. Chemical reactions start to consume both, the CO_2 residually trapped in the porous formation sandstone and the parts dissolved in the brine. Hence, mineralization of carbonates occurs along the CO_2 migration pathway as well as at the final location of the gaseous CO_2 phase in the reservoir (Fig. 4).

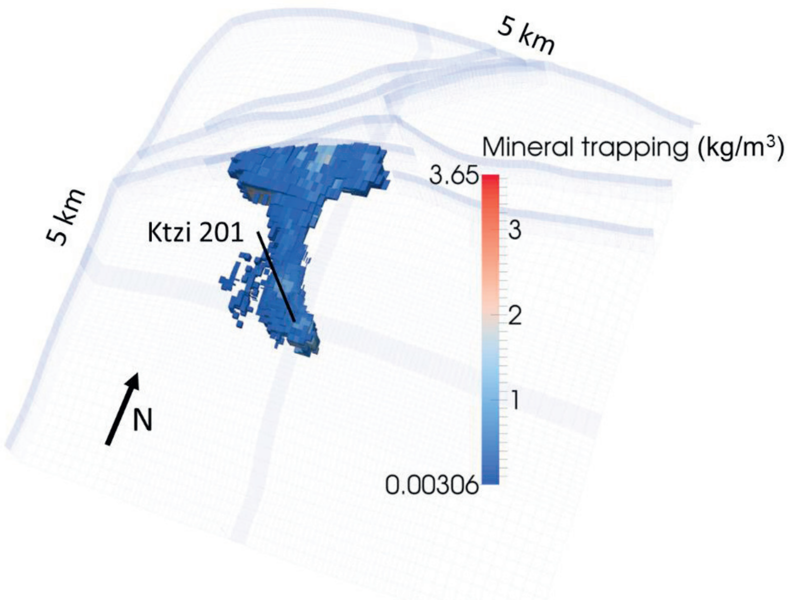

Fig. 4. Carbonate mineralization at the Ketzin pilot site in the Stuttgart Formation after 10.000 years based on the dynamic simulations [16].

Fig. 5 shows the time-dependent development of the four CO_2 trapping mechanisms suggested by the IPCC [15] (left) and calculated for the Ketzin pilot site (right). In the IPCC diagram, structural trapping is more dominant at one year after the injection stop and contributes to CO_2 trapping with 13.4 % after 10,000 years. However, the calculations for the Ketzin pilot site indicate that the relative amount of dissolved CO_2 is about twice as high already after one year, and that CO_2 dissolution is dominating the trapping mechanisms with 74 % to 81 % after 10,000 years. While the residual trapping contribution is increasing until about year 100 in the IPCC diagram, it is diminishing at the Ketzin pilot site throughout the entire 10,000 years of simulation. Consequently, structural and residual trapping are negligible at the Ketzin pilot site with a cumulative contribution of 1 % at 10,000 years after injection stop, but exhibit about 19 % in the IPCC diagram. Mineral trapping starts about 100 years later at the

Ketzin pilot site, but the calculated maximum trapping scenario (about 25 %) results in an order of fixed CO_2 almost comparable to that suggested by IPCC (about 37 %). The main reason for the dominating solubility trapping at the Ketzin pilot site is the CO_2 injection into the anticline flank followed by its upward migration along the reservoir top. This, in addition to the fluvial origin of the storage reservoir is expected to be responsible for a relatively large interface area between CO_2 and formation fluid compared to an e.g. marine sandstone reservoir with homogeneous reservoir properties. As a consequence, CO_2 dissolution is significantly higher. Furthermore, the CO_2 amount injected into the Stuttgart Formation at pilot-scale dimensions is far below the theoretical storage capacity of the Ketzin-Roskow anticline. Hence, the dissolved to gaseous CO_2 ratio would differ, if CO_2 would have been stored at industrial-scale dimensions.

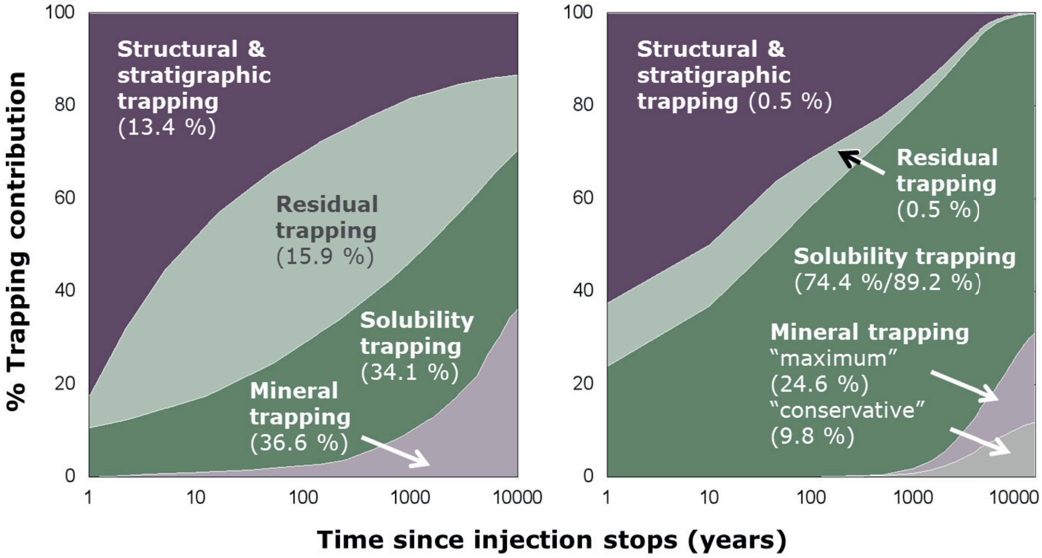

Fig. 5. Contribution of the four CO_2 trapping mechanisms to increasing storage safety after IPCC (2005) [15] (left) and predicted by coupled numerical simulations for the Ketzin pilot site [16,18] (contribution of each trapping mechanism at 10,000 years is given in the parentheses).

Mineral trapping of CO_2 at Ketzin is dominated by siderite, dolomite and magnesite, with start of significant precipitation after about 500 years after stop of injection. Mineralization continues until the end of the simulated period [16,18]. The total contribution of mineral trapping in the Stuttgart Formation at the Ketzin pilot site depends on the selected chemical constraints and ranges from 9.8 % to 24.6 %. At this time, almost all gaseous CO_2 (0.5 %) has been dissolved and residual trapping contributes by only 0.5 % to the total CO_2 mass balance. It is obvious that CO_2 dissolution is the most important trapping mechanism for long-term stabilization at the Ketzin pilot site with a contribution of 74.4 % to 89.2 % (Fig. 5).

Our results are in good agreement with the findings of the natural analogue study by Gilfillan et al. [34] indicating a maximum mineral trapping of 18 % with CO_2 dissolution in formation water being the main CO_2 sink in natural gas fields over geological time spans. Simulations of Audigane et al. [35] show comparable mineral assemblages with precipitates consisting of carbonates as e.g. siderite and calcite. In total, they receive an amount of 95 % dissolved and 5 % mineralized CO_2 after 10,000 years. Xu et al. [36,37] come to the conclusion that the major CO_2 trapping minerals are dawsonite and ankerite. However, this and the total capacity depend on primary mineral composition, whereby mineral trapping occurs in any case mainly within the reservoir sandstone. They also report precipitation of siderite and ankerite. The total mineralization within their simulated examples is on the order of 29 % after 1,000 years. The issues with dawsonite are not very well known and basic data needed for quantifying the respective chemical reactions. Different to many other reactive transport simulations, we disregarded in our case dawsonite which is quite often the major sink for CO_2. However, from Benezeth et al. [38] we deduce that Ketzin is not within the major stability field regarding CO_2 fugacity, pH and temperature, and therefore did not include it as a secondary mineral in our geochemical simulations. Nevertheless, it is furthermore expected that the trapping mechanism diagram (Fig. 5) is as well strongly site-specific depending on geological, geochemical and operational boundary conditions.

5. Conclusions

Long-term assessment of CO_2 storage sites requires, besides migration of CO_2, displacement of formation fluids and resulting pressure development in the reservoir, verification of geomechanical integrity and quantification of mineralization. For that purpose, we completely depend on the application of numerical simulation tools, because neither laboratory experiments nor field studies are able to answer the questions on the required spatial and temporal scale. Due to the computational effort, a fully coupled model of high spatial resolution covering thousands of years and taking into account hydraulic, thermal, chemical and mechanical processes cannot be conducted to date.

Given the fact that the relevant processes in a storage reservoir and its surrounding rocks contribute in a diverse way to the long-term behavior of CO_2 in the subsurface, we have developed a sophisticated workflow based on simplifications in the process coupling. Basis is the static geological model, which serves as input for multi-phase flow simulations. The results are fed into hydro-mechanical simulations on the one hand and geochemical reactions on the other.

The presented work aimed at quantification of the hydro-mechanical system integrity and long-term mineralization of the Ketzin pilot site for CO_2 storage in Germany. A multi-phase flow reservoir model served as basis for the process model coupling. The relevance of the processes flow, transport, chemical reactions and deformation strongly depends on the time scale, where we differentiated between site operation (few to 50 years), abandonment (few years) and (thousands of years). In our approach, process coupling is only carried out, if the related processes show a significant impact on the simulated time scale by means of CO_2 migration, dissolution, mineralization and hydro-mechanical effects in terms of potential impacts on reservoir rock, caprock and/or fault integrity.

Results of hydro-mechanical simulations are mainly of interest during the period of site operation, since relevant pore pressure changes in the reservoir are expected to occur during this phase only. Vertical displacements at the reservoir top of maximum 6 mm and at the ground surface of maximum 4 mm were determined by simulations. Furthermore, storage formation, caprock and fault integrity were verified by the coupled simulations and are maintained during the entire operational time of the Ketzin pilot site.

Hydro-chemical studies were taken to assess long-term CO_2 mineralization at the reservoir scale. CO_2 dissolution is the main trapping mechanism with a share of 74.4 % and 89.2 % with mineral trapping of carbonates on the order of 9.8 % to 24.6 %. Residual as well as structural trapping are negligible after 10,000 years of simulation with a contribution of 0.5 % each.

The integrated simulation of coupled processes allowed us to carry out a thorough assessment of long-term site stabilization at the Ketzin pilot site involving the investigation of the CO_2 trapping mechanism contribution as well as of system integrity, whereby coupling of specific process models was undertaken depending on the process influence at the relevant time scales. We conclude that the entire system integrity is maintained after abandonment and in the long-term. The conceptual approach presented here can be easily adapted to and applied at other CO_2 storage sites as well as geological reservoirs world-wide.

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