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Assessment of long-term CO_2 trapping mechanisms at the Ketzin pilot site (Germany) by coupled numerical modelling

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Abstract
To assess the long-term reservoir stabilisation at the Ketzin pilot site (Germany), the contribution of the four CO_2 trapping mechanisms (structural, residual, dissolution and mineralisation trapping) was determined by numerical modelling. In the first step, dynamic flow simulations were undertaken using a reservoir simulator. The second step comprised batch simulations applying a geochemical simulator. Coupling between both simulators was achieved by time-step dependent integration of water saturation calculated in the reservoir simulations. After a simulation time of 16,000 years, about 98.3 % of the injected CO_2 is dissolved in the formation fluid and 1.5 % mineralised, while residual trapping contributes with 0.2 % and structural trapping is negligible.

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Keywords: CO_2 storage;CO_2 trapping mechanisms;Ketzin pilot site; brine displacement; numerical modelling

1. Introduction

The Ketzin pilot site located in Germany is the first European on-shore site for CO_2 storage [1] [2] [3] [4] [5]. CO_2 injection was started in June 2008 with about 61,000 tonnes of CO_2 injected until today (October 2012). The storage formation (Stuttgart Formation, Middle Keuper, Triassic) has an average thickness of about 74 m and is determined by fluvial facies, whereby high-permeable sand channels dominate the multi-phase flow regime in the reservoir and provide a net thickness of about 18 m in the vicinity of the injection well (Ktzi 201) and three observation wells (Ktzi 200, Ktzi 202 and Ktzi 203). Recent updates of the geological model which general implementation is discussed by Norden and Frykman [6] allowed to revise the partially successful history match undertaken by Kempka et al. [7] and match the simulations with regard to Ktzi 201 and Ktzi 202 bottom hole pressure 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 deviations of below 10 % [4] [8].

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The contribution of the four CO_2 trapping mechanisms was determined for the Ketzin pilot site in two separate steps. In the first step, reservoir modelling was undertaken using the Schlumberger ECLIPSE 100 black-oil reservoir simulator [9] adapted for CO_2 storage as introduced in Kempka et al. [7]. The reservoir simulations presented here use the latest version of the history matched reservoir model and were conducted for a simulation time of 16,000 years to account for the long-term development of trapping mechanisms. The second step of our approach comprised geochemical batch simulations using the PHREEQC simulator [10] the dissolved CO_2 mass and water saturation determined by the reservoir simulations previously undertaken. The coupling scheme introduced by Klein et al. [11] was used in the present study to combine the reservoir simulation results with subsequent geochemical batch simulations to quantify the contribution of each trapping mechanism to long-term site stabilisation.

2. Reservoir simulations to determine long-term structural, residual and solubility CO_2 trapping

Reservoir simulations parameterised as discussed by Kempka et al. [7] and Kempka and Kühn [8] were performed for a time-span of 16,000 years using the latest version of the reservoir model with a lateral size of 5 km x 5 km and an average thickness of about 74 m. The applied reservoir model incorporates seven faults at the top of the Ketzin anticline open for cross-flow but not allowing for vertical flow along the fault planes. These assumptions are supported by present knowledge on the operation of the former natural gas storage site in the Jurassic. Figure 1 shows the spatial discretisation of the reservoir model and its near-well area (5 m x 5 m) with the three wells Ktzi 201, Ktzi 200 and Ktzi 202, respectively. The vertical discretisation of the reservoir model is represented by three zones with 60 layers, whereby the uppermost zone (about 25 m thickness) has a vertical discretisation of 0.5 m increasing in the two zones below. 648,420 active elements were used to represent the storage formation, whereby local grid refinements (LGR) were not applied in order to maintain a structured grid for the sake of compatibility with other simulation codes.

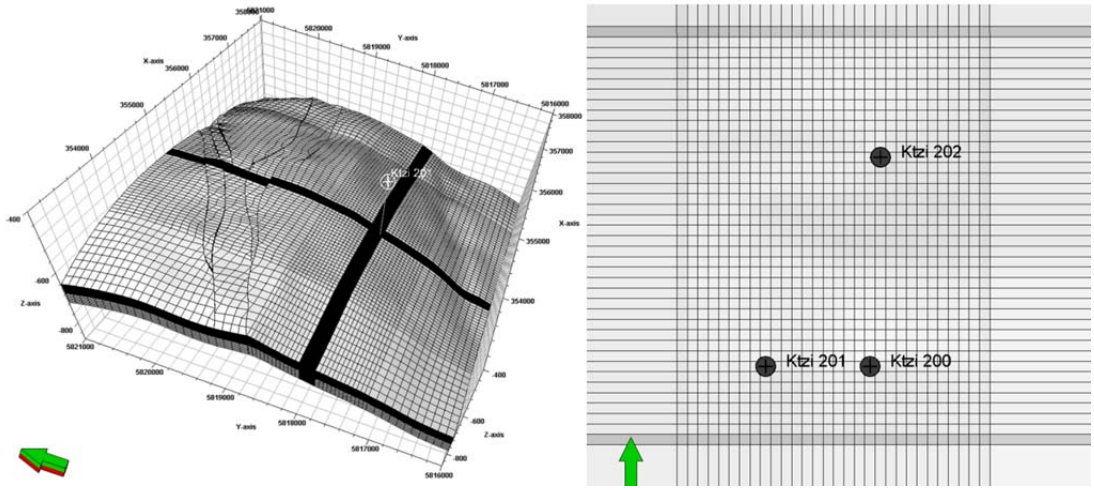

Figure 1: Ketzin pilot site reservoir model of the Stuttgart Formation with seven faults at the anticline top and its spatial discretisation with 648,420 active elements (left) and near-well horizontal discretisation (5 m x 5 m) with locations of Ktzi 201 injection well as well as Ktzi 200 and Ktzi 202 observation wells (right).

Seven faults penetrating the entire reservoir thickness at the top of the Ketzin anticline indicate the graben structure with vertical offsets of 10 m to 20 m. Here, cross-flow is only possible at locations where high-permeable facies (sand channels) are in contact with each other across the fault, since transport in

the low-permeable flood-plain facies is mainly limited to diffusive processes. A pore volume multiplier of 10,000 was applied at the boundary elements of the modelling domain to simulate an infinite aquifer corresponding to the observations made at the Ketzin pilot site. The Ketzin pilot site injection regime from June 2008 until December 2011 [12], unpublished data on site operation (available until May 2012) as well as the latest operational schedule valid until the end of injection operation in June 2013 were considered in the reservoir simulations, whereas site abandonment is expected to start after June 2013. From that time on, CO_2 migration and long-term site stabilisation were investigated up to the year 18,000 (about 16,000 years of simulation time).

The volume of structurally trapped CO_2 at standard conditions was calculated according to the presence of a gaseous CO_2 phase volume (V_{CO_2}) in the related element of the reservoir model and subsequently reduced by the amount of CO_2 residually trapped ($V_{CO_2,r}$)in that element (cf. Equation 1). Here, S_g is the gas saturation and S_{gr} the residual gas saturation of the related element considered to be constant at 0.05 in the entire reservoir model. Solubility trapping was determined according to the ratio of CO_2 dissolved in the formation fluid.

$$V_{CO_2,r} = \begin{cases} \frac{S_{gr} \cdot V_{CO_2}}{S_g}, & S_g > S_{gr} \\ V_{CO_2}, & S_g \leq S_{gr} \end{cases}, \text{ where } S_{gr} = 0.05 \qquad \text{(Equation 1)}$$

Figure 2 shows the spatial distribution of gaseous CO_2 at different simulation times from the stop of injection in 2013 up to the year 18000. The CO_2 plume continues to migrate dip-upward, whereas the flow in NWN direction is dominated by the distribution of the high-permeable sand channels in the Stuttgart Formation. From 2013 to 2100 the amount of gaseous CO_2 is being significantly reduced by dissolution in the formation fluid. A free gas cap establishes close to the anticline top hindered by the fault offset to migrate to its topographical top in year 4500. Here, a low gaseous CO_2 saturation may be still observed in the vicinity of the injection well, which is being dissolved until the year 12000. At the final simulation tine (year 18000) almost all gaseous CO_2 migrated to the anticline top is dissolved, and thus the gas cap is almost diminished.

Timely development of spatial distribution of the CO_2 saturated formation fluid (sm^3 CO_2/sm^3 brine) is illustrated in Figure 3. As expected, the highest saturations of dissolved CO_2 appear in the vicinity of highest CO_2 gas phase saturations and accompany the dip-upward plume migration from 2013 to 2100). While the free gas cap develops at the anticline top from 2100 to 7000, high saturations of dissolved CO_2 are being continuously reduced by diffusion processes triggering a vertical extension of the CO_2 saturated formation fluid. This process continues from years 12000 to 18000, whereby almost all CO_2 injected is dissolved in the formation fluid (99.8 %) at the final time step. The fraction of gaseous CO_2 (structural trapping) is negligible at the end of the simulation time, but residual trapping still amounts to 0.2 %.

3. Geochemical simulations to determine CO_2 mineralisation and coupling to reservoir simulations

To quantify long-term mineral trapping geochemical modelling was performed for a simulation time of 16,000 years. Fluid and mineral composition were provided by site-specific core and fluid sample analysis as summarized in Klein et al. [11]. Primary rock-forming minerals introduced into the model are K-feldspar, albite, illite, chlorite, anhydrite and hematite. The formation fluid is strongly sodium chloride dominated with total dissolved solids (TDS) of about 237 g/l. To be consistent with the analytical brine composition, partial equilibrium with primary minerals was assumed.

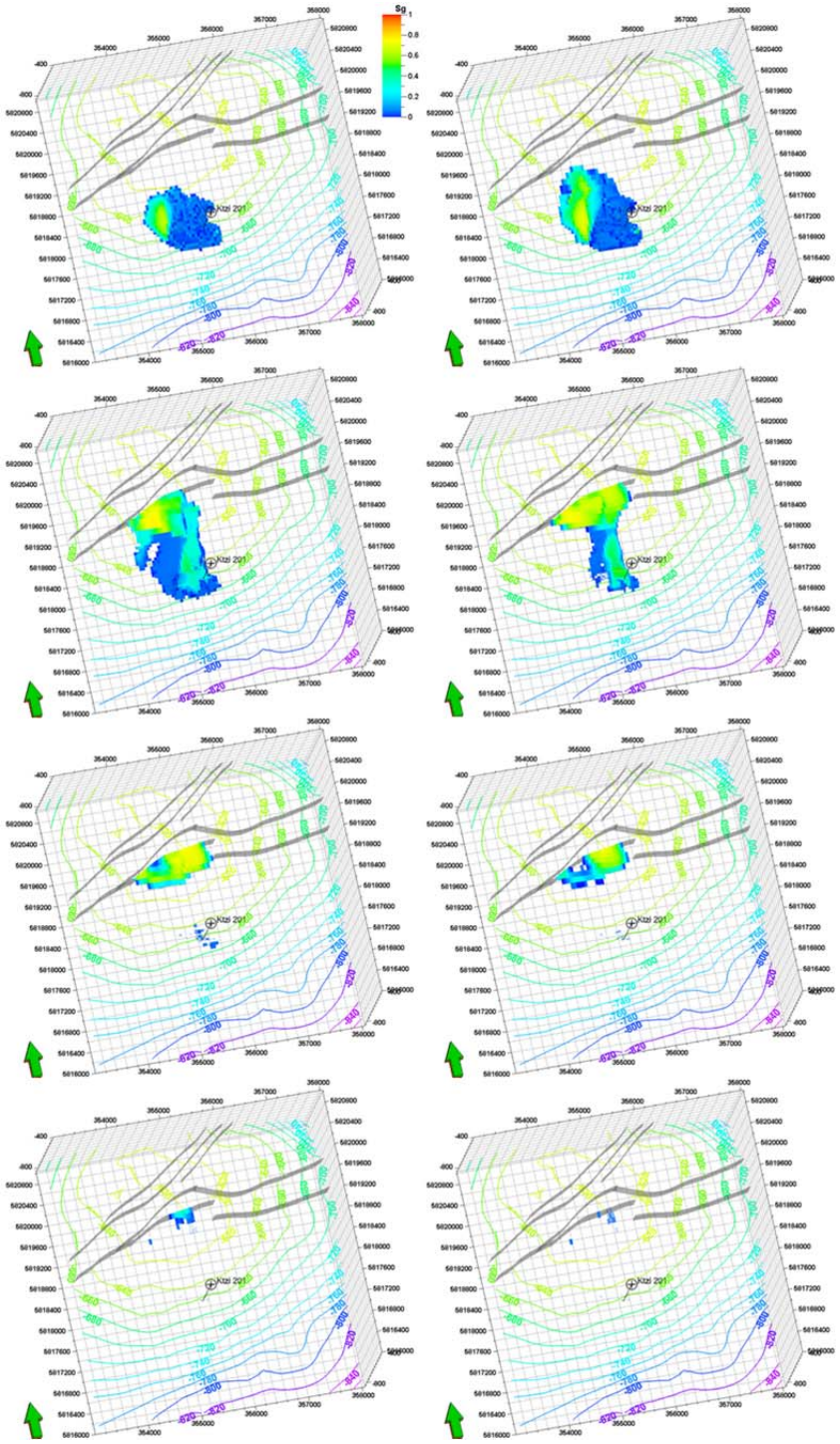

Figure 2: Gaseous CO_2 (CO_2-rich phase) saturation in the years 2013 (after stop of injection), 2020, 2100, 2500, 4500, 7000, 12000 and 18000 (from left to right).

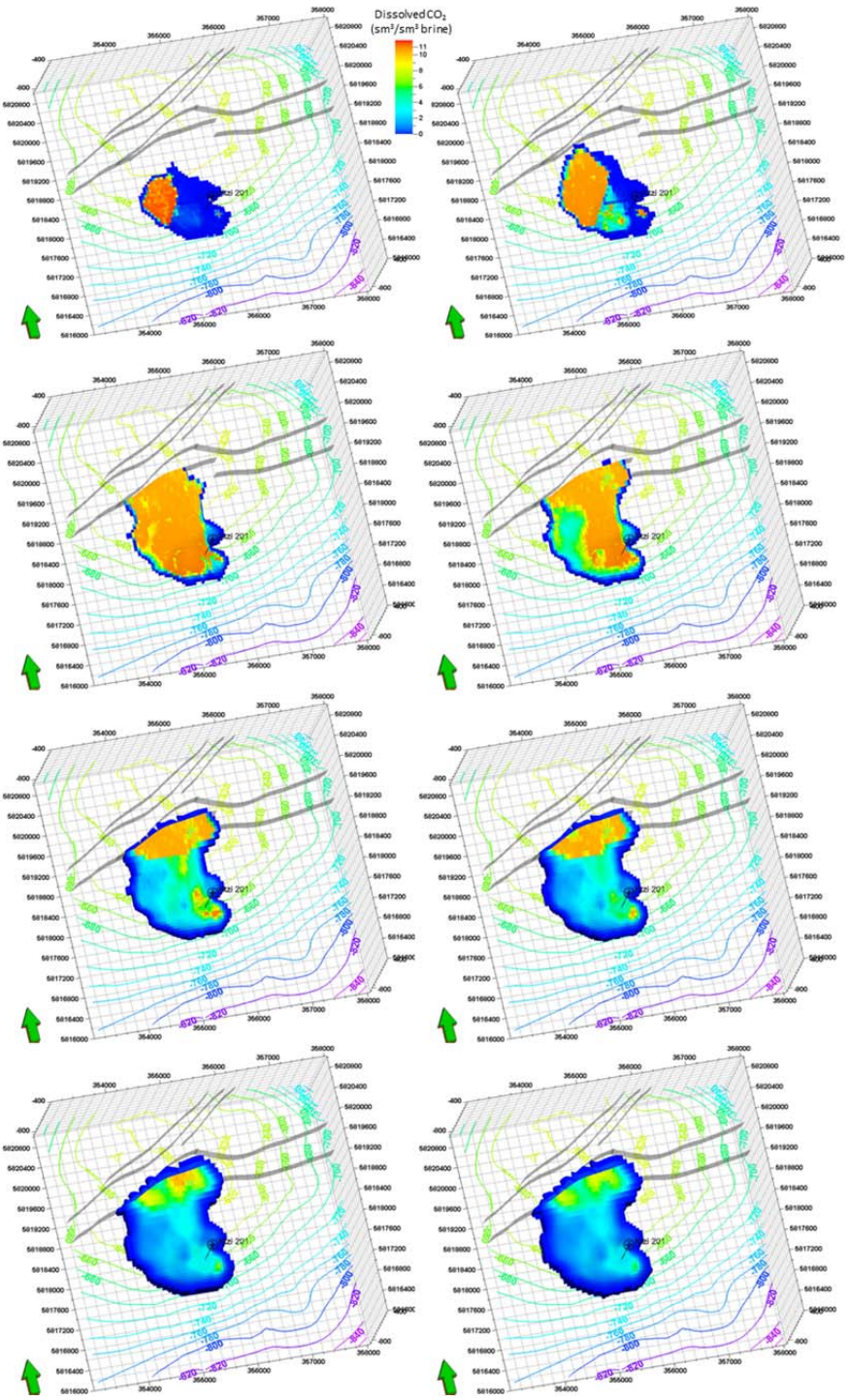

Figure 3: CO_2 dissolved in the formation fluid in the years 2013 (after stop of injection), 2020, 2100, 2500, 4500, 7000, 12000 and 18000 (from left to right).

Secondary minerals were selected analysing the saturation index of all minerals present in the thermodynamic database (LLNL) after imposing equilibrium among the primary mineral assemblage, brine and CO_2. According to that, calcite, dolomite, kaolinite, magnesite, pyrite and siderite were introduced as secondary minerals. Except for calcite and anhydrite, which were assumed to be at local equilibrium, dissolution and precipitation of minerals were simulated under kinetic conditions.

Various geochemical simulations were performed for different porosity and water saturation scenarios covering the observed range of 8 to 24 % porosity and 40 to 100 % water saturation based on the reservoir simulations in the reservoir. In all cases, there is an increase of mineral trapping in time which was consecutively taken over by siderite, dolomite and magnesite. With growing porosity precipitation occurred slower but in a larger amount. Results also indicated a scalability of mineral trapping for different porosities and water saturations, whereby the analytical scaling relationship is provided and discussed in Klein et al. [11]. Being able to consider heterogeneous porosity and water saturation scenarios based on one single simulation run was fundamental for the coupling strategy of geochemical and reservoir simulations.

Coupling of geochemistry to reservoir simulations required some considerations and hypothesis to be made. To account for the boundary conditions of the geochemical model, strict criteria were applied for the selection of the elements of the reservoir simulation grid in which geochemistry can be considered active. First, the starting point of CO_2 exposure, the total time of CO_2 exposure, the average water saturation during that time and the porosity were evaluated for each element. Then, all elements in which a CO_2-rich gas phase was present and whose porosity within the range of 8 to 24 % were selected as contributing to mineral trapping. In the geochemical simulations it is assumed that dissolved CO_2 is at equilibrium with a constant pressure of the CO_2 gas phase in contact with the solution. Elements with zero gas saturation do not fulfil this boundary condition and were therefore neglected. Under the described conditions, only 3% of the volume being occupied by CO_2 (either dissolved or as a gas) after 16,000 years was considered for quantification, resulting in a final mineralisation of 1.5 % of the total injected CO_2. Since only dissolved CO_2 may participate in geochemical processes, it is required to maintain the CO_2 balance of the reservoir model by reducing the amount of dissolved CO_2 by that of the mineralised.

4. Contribution of CO_2 trapping mechanisms to long-term stabilisation at the Ketzin pilot site

Figure 4 shows the timely development of the four CO_2 trapping mechanisms investigated for the Ketzin pilot site as a result of the reservoir and geochemical model plotted in the style of the well-known IPCC [13] diagram. At the Ketzin pilot site, about 62 % of CO_2 is structurally trapped after six years of injection (June 2008 to June 2013) with a cumulative amount of about 68,800 t of CO_2. Furthermore, about 24 % of CO_2 is dissolved in the formation fluid and 14 % residually trapped at that time, while CO_2 mineralisation does not occur in the first 500 years of simulation.

During the following dip-upward migration residual CO_2 trapping does not increase, since diffusion dominates the dissolved CO_2 ratio in the formation fluid supporting fast dissolution in brine undersaturated with CO_2.

For a more detailed understanding of the pressure drop in the reservoir (cf. Figure 5, right), timely development of formation fluid displacement has to be considered. When injection stops after five years in 2013, about 135,816 sm^3 of brine have been displaced into the large volume boundary elements applied for infinite aquifer implementation as plotted in Figure 5 (left).

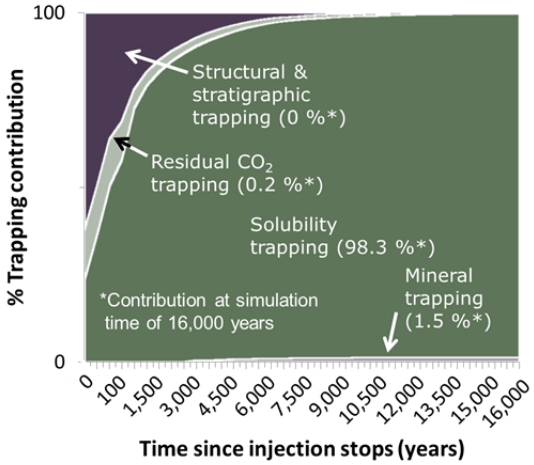

Figure 4: Contribution of the four CO_2 trapping mechanisms at the Ketzin pilot site for a time-span of 16,000 years predicted by coupled numerical simulations.

Brine displacement can be observed until about 15 years of simulation, while gaseous CO_2 is migrating dip-upward and its volume expanding. Furthermore, brine displacement and formation of a gas cap at the anticline top impose a pressure decrease below initial reservoir conditions (60.1 bar) by about 1.2 bar at the Ktzi 202 well (cf. Figure 5, right) with a maximum of 0.31×10^6 sm^3 brine displaced vs. an injected CO_2 volume of 36.9×10^6 sm^3. In the following simulation time, volume expansion is hindered due to negligible pressure changes as the CO_2 plume is not able to migrate beyond the fault offset boundary at anticline top. In addition, CO_2 dissolution strongly contributes due to the increased contact area of gaseous CO_2 and brine (cf. Figures 2 and 3). Progressive development of CO_2 dissolution (cf. Figure 4) triggers a volume decrease of the gaseous CO_2 cap and allows for backflow of brine from the boundary elements. In year 18000, a total amount of 0.04×10^6 sm^3 brine still remains displaced (cf. Figure 5, left) and pressure is equilibrated back to the initial reservoir conditions (cf. Figure 5, right).

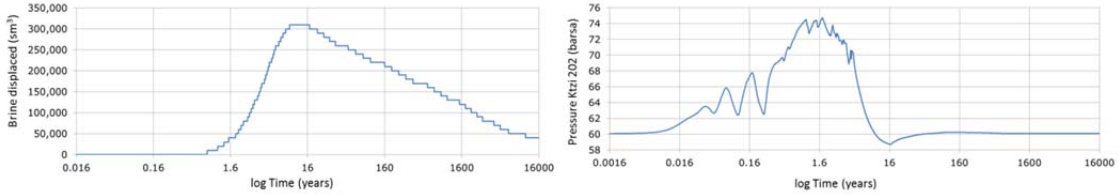

Figure 5: Brine displacement during entire injection and long-term site stabilisation up to 16,000 years of simulation time. A maximum brine displacement of 310,000 sm^3 is achieved after about 15 years and reduced to about 40,000 sm^3 by brine backflow after 16,000 years (left). Ktzi 202 observation well bottom hole pressure during entire simulation time of 16,000 years showing the pressure effect of brine displacement and its backflow starting after about 16 years of simulation until achievement of long-term site stabilisation (right).

Mineral trapping of CO_2 is dominated by the minerals siderite, dolomite and magnesite, whereas precipitation starts about 500 years after stop of injection and continues until the end of the simulation time [11]. The total contribution of mineral trapping in the Stuttgart Formation at the Ketzin pilot site is relatively low with about 1.5 % in year 18,000 (16,000 years of simulation time). At this time, almost all gaseous CO_2 has been dissolved and structural trapping contributes by 0.2 % to the entire CO_2 trapping mass balance. Consequently, CO_2 dissolution can be identified as the most important trapping mechanism for long-term stabilisation at the Ketzin pilot site.

5. Conclusions

We presented the assessment of the contribution of the four CO_2 trapping mechanisms (structural, residual, solubility and mineral trapping) to long-term stabilisation at the Ketzin pilot site (Germany). A two-step numerical modelling approach was applied to predict the long-term processes in the storage formation, whereby structural, residual and solubility trapping were computed using a reservoir simulator subsequently coupled to a geochemical batch simulator to account for CO_2 mineralisation. Simulation results show that after a simulation time of 16,000 years (year 18000), about 98.3 % of the injected CO_2 is dissolved in the formation fluid and 1.5 % mineralised, whereas residual trapping accounts to 0.2 % and structural trapping is negligible at the Ketzin pilot site. The resulting IPCC-like plot on trapping mechanisms at the Ketzin pilot site (cf. Figure 4) shows significant deviations to the original IPCC diagram [13]. This emphasises that CO_2 trapping mechanisms are site-specific and strongly depend on local P/T conditions, structural topography and injection well placement as well as fluid and rock geochemistry amongst other geological boundary conditions.

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