SPECIAL ISSUE

Numerical simulations of CO_2 arrival times and reservoir pressure coincide with observations from the Ketzin pilot site, Germany

Thomas Kempka · Michael Kühn

Abstract Numerical simulations of CO_2 migration for the period June 2008–December 2011 were performed based on a unique data set including a recently revised static geological 3D model of the reservoir formation of the Ketzin pilot site in Brandenburg, Germany. We applied the industrial standard ECLIPSE 100 and scientific TOUGH2-MP simulators for this task and implemented a workflow to allow for integration of complex model geometries from the Petrel software package into TOUGH2-MP. Definition of a near- and a far-field well area allowed us to apply suitable permeability modifiers, and thus to successfully match simulation results with pressure measurements and arrival times in observation wells. Coincidence was achieved for CO_2 arrival times with deviations in the range of 5.5–15 % and pressure values in the injection well CO2 Ktzi 201/2007 and the observation well CO2 Ktzi 202/2007 with even smaller deviations. It is shown that the integration of unique operational and observation data in the workflow improves the setup of the geological model. Within such an iteration loop model uncertainties are reduced and enable advanced predictions for future reservoir behaviour with regard to pressure development and CO_2 plume migration in the storage formation at the Ketzin pilot site supporting the implementation of monitoring campaigns and guiding site operation.

Keywords Numerical modelling · CO_2 storage · Ketzin pilot site · ECLIPSE · TOUGH2

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Introduction

The Ketzin pilot site located in the State of Brandenburg, Germany, was the first European on-shore site for CO_2 storage in a saline aquifer and is now operated for >4 years (Martens et al. 2012; Würdemann et al. 2010). So far, three wells (CO2 Ktzi 201/2007 for injection and observation as well as CO2 Ktzi 200/2007 and CO2 Ktzi 202/2007 for observation) have been drilled down to the base of the Stuttgart Formation in 800 m depth in the Keuper. The target formation for CO_2 injection is at a depth of about 630–650 m at the injection well CO2 Ktzi 201/2007. CO_2 has been injected since June 2008 at an average rate of about 0.5 kg/s based on an injection schedule considering different monitoring campaigns, well tests and operational revisions. Operational data for the Ketzin pilot site were recently published by Möller et al. (2012) covering all relevant data for simulations from the start of injection up to the end of the year 2011.

The scientific novelty elaborated in the study presented here is based on a wide range of geological and monitoring data from the Ketzin pilot site. Compared to other locations around the world, breadth and depth of the measurements and longevity of the recorded time series are unique as shown by Michael et al. (2010) and references therein. This enables us to parameterise with great detail our static geological and dynamic flow models (e.g. Norden and Frykman 2013). Characteristic for that beside others is the permanent bottom hole pressure measurement and monitoring. From that perspective the available data set is unique because only the pilot sites like Ketzin, Frio, Nagaoka and Otway do have bottom hole pressure data (Michael et al. 2010). The larger demonstration projects of Sleipner or In Salah are lacking that. The pilot sites Frio and Nagaoka are orders of magnitude smaller compared to

Ketzin with regard to the amount of injected CO_2. Otway is of the same size, however, it is a pilot for CO_2 storage in a depleted gas field. It is only Ketzin which can provide bottom hole pressure data to be used for dynamic model matching for a time-span of >4 years (Möller et al. 2012) and a significant amount of injected CO_2 into a saline aquifer (Martens et al. 2012). Taking into account the high complexity of the geological setting of the fluvial Stuttgart Formation and the monitoring data density (especially related to pressure profiling) a sufficiently good match of bottom hole pressure in acceptable agreement with CO_2 arrival times in the observation wells offers an excellent, unique and new opportunity to validate the numerical simulation tools currently available.

Kempka et al. (2010) discussed predictive models for CO_2 injection at the Ketzin site. These simulations were based on the static geological 3D model available at that time which did not include the interpretation of the 3D seismic repeat from late October 2009. All available geophysical and geological information is used for recurring updates of the static model. In 2010, Kempka et al. determined that the simulated CO_2 arrival at the first observation well (CO2 Ktzi 200/2007) can be matched with deviations of 21–33 % in the predictive case and 8.1–17.7 % applying the actual injection regime neglecting the pressure development in the reservoir. It was therefore concluded that knowing the injection regime is of utmost importance to be able to predict the CO_2 migration in the reservoir more accurately. The arrival time of the CO_2 at the second observation well (CO2 Ktzi 202/2007) could not be matched by any of the applied codes, indicating that the geological model did not represent the actual geological conditions at that time. Hence, complete coincidence between monitoring and modelling with the previous static geological 3D model could not be gained with regard to reservoir pressure and arrival times. Considering these simulation results, Lengler et al. (2010) employed a Monte Carlo analysis to assess heterogeneity in porosity and permeability by means of representing a potential driver for the late CO_2 arrival observed at the CO2 Ktzi 202/2007 well. They demonstrated that heterogeneity is very unlikely responsible for the deviation in CO_2 arrival time at the second observation well. Through these findings and supported by updates in monitoring data, the geological model was revised by implementation of a facies-based heterogeneity in the CO2 Ktzi 202/2007 near-well area consisting of floodplain and sand channel facies with low and high permeabilities, respectively, as discussed in Kempka et al. (2013b).

Updates of monitoring data obtained by 3D seismic (re-)interpretation, electrical resistivity tomography and well logging allowed for a revision of the initial static geological model which is presented by Norden and

Frykman (2013). The latest geological model revision (Kempka et al. 2013b) is employed for the reservoir simulations presented in this study.

We expected now a better match between observations and simulations based on the revised static geological 3D model independent of the application of two different simulators. We wanted to show that integration of new observation data improves the quality of a static geological model significantly to better match observation data with each iteration. The presented work is a continuation from Kempka et al. (2010), whereas dynamic flow coupled with geochemical simulations accounting for CO_2 trapping mechanisms are discussed in Klein et al. (2013), Kempka et al. (2013a) and Fischer et al. (2013). Here, the industrial standard simulator ECLIPSE 100 (Schlumberger 2009) and the scientific simulator TOUGH2-MP/ECO2N (Zhang et al. 2008; Pruess 2005) were applied for this unique dynamic flow simulation study. An extended simulator intercomparison study using the Ketzin pilot site static geological model and monitoring data is presented in Kempka et al. (2013b).

Model setup and parameterisation

Model geometry and discretisation

The implementation of the initial static geological 3D model of the Ketzin anticline is described in detail by Norden and Frykman (2013). Meanwhile, observation data available for a period until the end of 2011 has been integrated into the geological model (3D seismic (re-)interpretation, electrical resistivity tomography and well logging) in addition to updated operational data (pressures and injection rates). The geological model has a lateral size of 5 × 5 km and a thickness of about 72 m also involving seven major faults with the respective offsets at the top of the anticline. In the first step, we up-scaled the reservoir properties relevant for dynamic simulations (effective porosity, permeability and facies description) from the initially very fine geological grid of 5 × 5 m lateral size to the grid of our reservoir model illustrated in Fig. 1 using the Petrel 2010 software package (Schlumberger 2010). For that purpose, we defined three lateral zones of different discretisation: a near-well zone of 150 × 200 m and 5 × 5 m element size (Fig. 2); a zone considering the size of the expected CO_2 plume for the envisaged simulation time of 3.5 years of 3.5 × 1.5 km and 50 × 50 m element size (Fig. 3); and an outer zone (5 × 5 km) with 100 × 100 m element size (Fig. 3). The initial vertical discretisation applied in the revised geological model consists of three zones (Zone A: about 24 m thickness with 0.5 m elements, Zone B: about 12 m
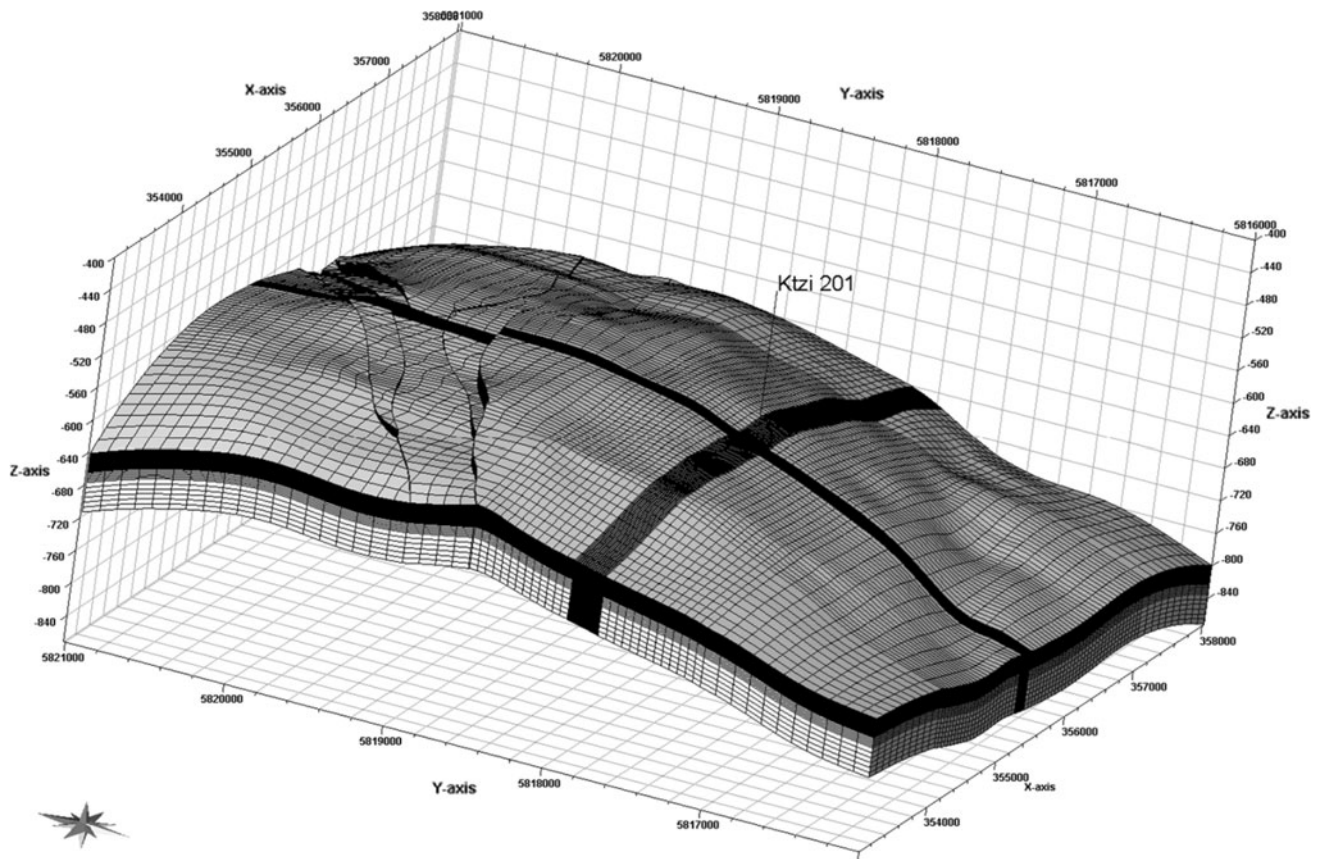
Fig. 1 3D view of the reservoir model of the Ketzin anticline (5 × 5 km × about 72 m) with three different lateral and vertical discretisation zones and seven major faults at the top of the anticline (vertically exaggerated by factor 5)

thickness with 1 m elements and Zone C: about 36 m thickness with 3 m elements) was up-scaled to 2 m elements in Zone B and 6 m elements in Zone C, while vertical discretisation in Zone A was not modified to account for buoyancy effects of the multi-phase system by a sufficient vertical resolution of the uppermost layers (Fig. 1). The resulting reservoir model consists of 648,420 active elements discretised by 107 elements in i-, 101 elements in j- and 60 elements in k-direction.

Model parameterisation

We developed a workflow allowing for a conversion of Petrel data sets into the TOUGH2-MP/ECO2N input data format that was applied in order to ensure identical implementation in terms of geometry, discretisation and properties of the reservoir model in both simulators applied. This workflow comprises multiple steps beginning with reading in of the initial reservoir simulation structured hexahedron grid constructed using an arbitrary pre-processing software package (e.g. Schlumberger Information Services Petrel) and its storage in an adapted data structure representing element ids,

corner coordinates, centres and volumes determined according to the approach of Grandy (1997). Additional information such as, the connection distance, volume, interface area to other lateral and horizontal neighbouring elements are directly written into the TOUGH2-MP output file. Further pre-processing tools are applied to define initial and boundary conditions.

Parameterisation of the ECLIPSE and TOUGH2 models was done as discussed in Kempka et al. (2010) considering the following revisions:

- ranges of effective porosities and initial permeabilities as presented by Norden and Frykman (2013) were updated based on the latest observations at the Ketzin pilot site (Kempka et al. 2013b);
- initial permeability anisotropy was determined as $K_v/K_h = 1/3$, while the final permeability anisotropy was determined by matching observation and simulation data;
- initial pressure is 62 bar at a depth of 639.5 m in the CO_2 Ktzi 201/2007 well and temperature is considered to be constant at 34 °C in the entire reservoir (unpublished data);
- brine salinity is 0.22 kg NaCl equivalents per kg brine;

Fig. 2 Planar view of near-well discretisation applied in the reservoir model with the CO2 Ktzi 201/2007 injection as well as the CO2 Ktzi 200/2007 and CO2 Ktzi 202/2007 observation wells in about 50 and 112 m distance from the CO2 Ktzi 201/2007 well, respectively. Near-well lateral element size is 5×5 m
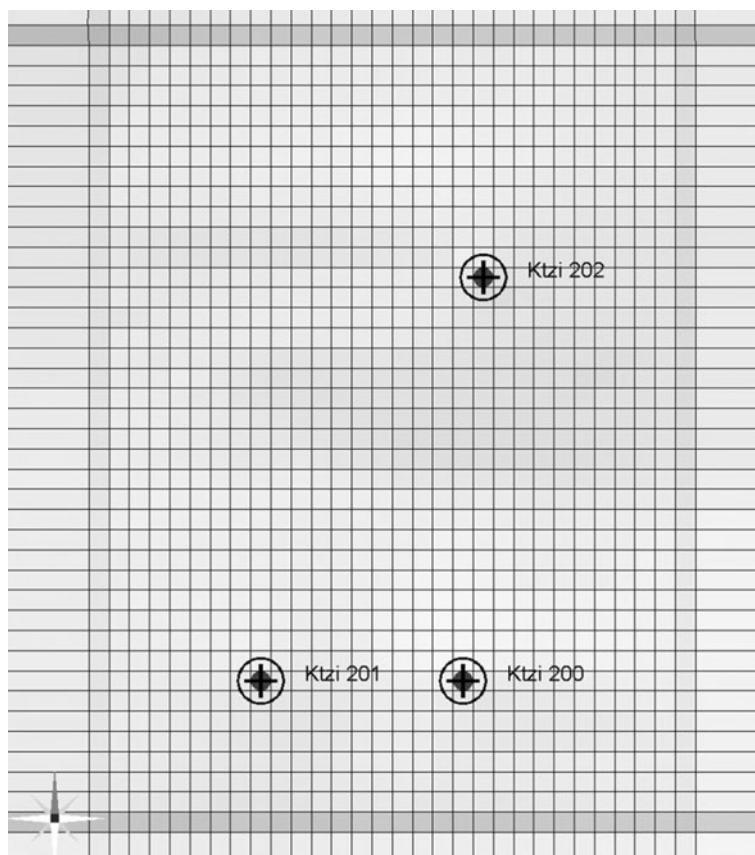
- the skin factor is neglected as it does not notably influence the simulation results;
- residual water saturation is $S_{wr} = 0.15$ and residual gas saturation $S_{gr} = 0.05$ as determined in laboratory experiments (unpublished data);
- relative permeabilities as well as capillary pressure were derived from flow-through experiments on core samples from the Stuttgart Formation (unpublished data). The input data for both simulators are illustrated in Fig. 4.

The seven major faults at the top of the Ketzin anticline were not implemented in the previous model (Kempka et al. 2010). As there is no indication of low horizontal fault permeability based on hydraulic tests undertaken (Wiese et al. 2010) and unpublished operational data of the gas storage operation, all seven faults implemented in the reservoir model were assumed to be horizontally conductive for fluid flow. According to permanent pressure and isotope monitoring in an indicator horizon located in the Exter Formation (about 180 m above the Stuttgart Formation), regional communication between that indicator horizon and aquifers in the Jurassic or the Stuttgart Formation may exist (Wiese et al. 2013). However, there is no evidence of CO_2 or brine migration from the Stuttgart Formation via the faults present at the anticline top.

Consequently, we defined all faults to be impermeable in vertical direction. Integrity of the upper (Weser Formation) and lower caprocks (Grabfeld Formation) are considered by no-flow top and bottom boundary conditions, while an infinite aquifer is accounted for by a (pore) volume multiplication factor of 10,000 at the lateral boundary elements to avoid boundary pressure effects.

The well implementation differs in both simulators as TOUGH2 does not come with a wellbore module, while ECLIPSE does. Hence, a simplified approach was chosen in the TOUGH2 simulations by assigning a high porosity of 0.99 and permeability of 1,000 mD to the cell column representing the well instead of the data derived from upscaling. ECLIPSE uses the original element porosities and permeabilities of the element column penetrated by the well, since the internal wellbore flow module can be applied. Open sections of the three wells (filter screens) at reservoir depth could be implemented identically in both models according to operational data (unpublished data).

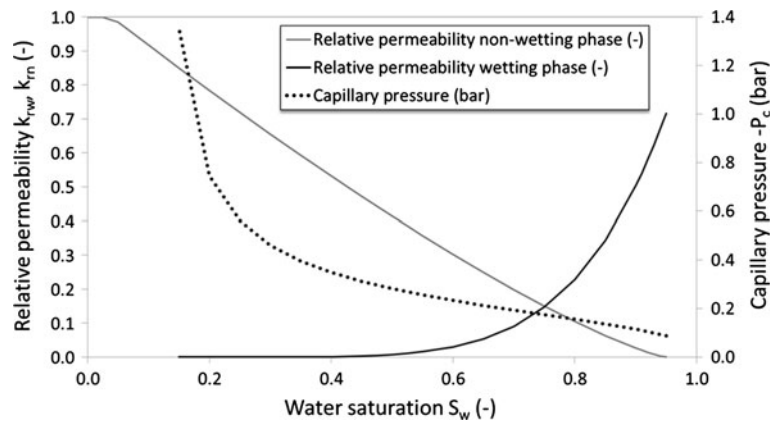Pressure correction and injection rate

CO_2 injection rates as well as temperature and pressure measured at 550 m depth in the CO2 Ktzi 201/2007 well from the start of injection until the end of 2011 are derived
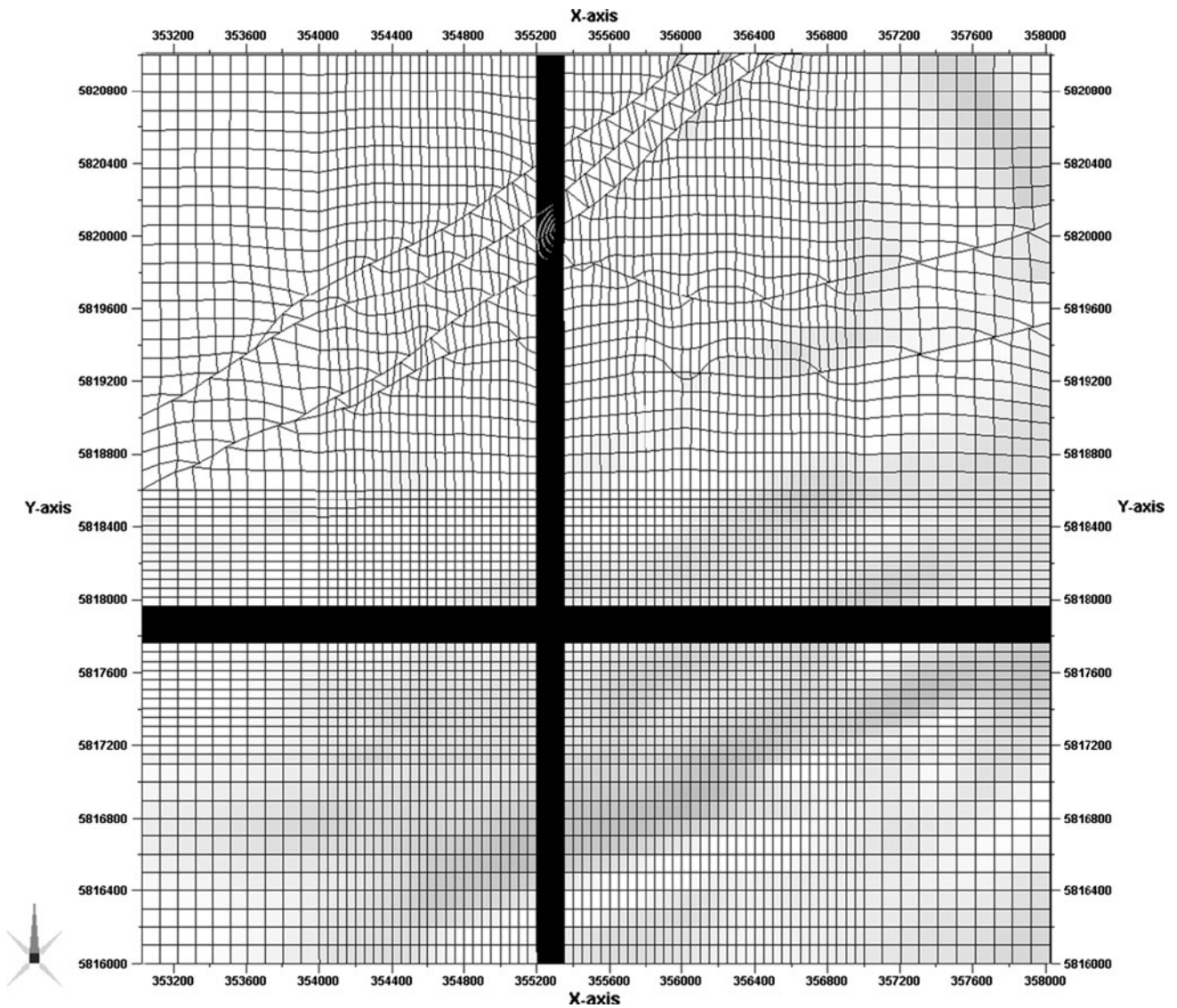
Fig. 3 Planar view of the different discretisation zones accounting for the near-well area (150 × 200 m), the expected CO$_2$ plume size at the envisaged simulation time (3.5 × 1.5 km) and the outer zone (5 × 5 km)

Fig. 4 Relative permeabilities for the wetting (k_{rw}) and non-wetting phases (k_{rn}) as well as capillary pressure determined by laboratory experiments and smoothened in order to assure convergence behaviour in the applied numerical simulators
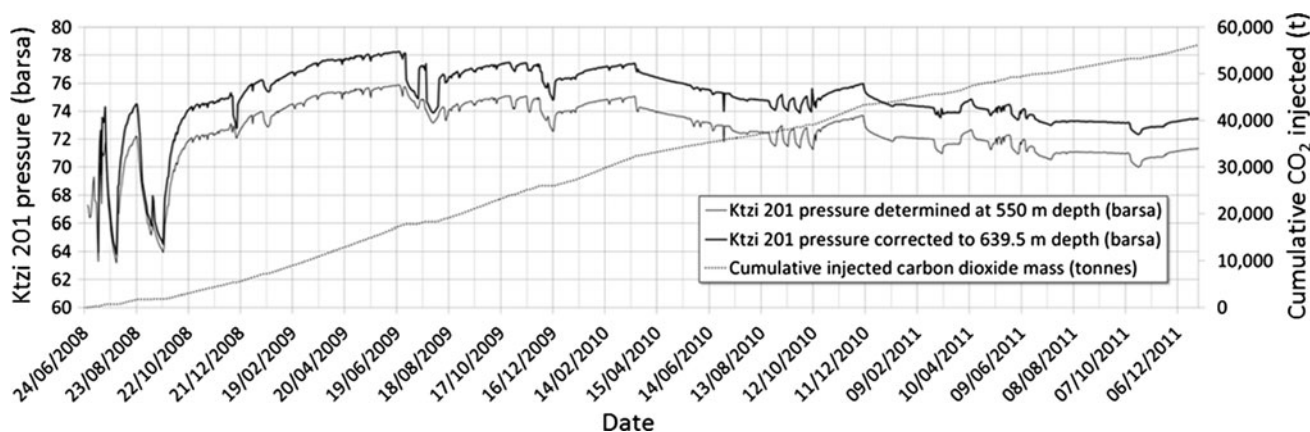
Fig. 5 Pressure measured in the injection well CO2 Ktzi 201/2007 at 550 m and cumulative injected CO_2 mass after Möller et al. (2012) as well as pressure corrected to the reference depth of 639.5 m

from Möller et al. (2012). Since the top of the reservoir is located about 80 m below the pressure and temperature sensor installed in the CO2 Ktzi 201/2007 well, a pressure correction to reservoir depth had to be applied to allow us for a comparison of simulation results and observed reservoir pressure. For that purpose, a density-based approach was chosen by discretising the vertical well section (89.5 m to the reference depth of 639.5 m) into vertical elements of arbitrary size and cumulating the pressure-dependent CO_2 density (and N_2 density during injection stops in the first year of operation) as a function of pressure and temperature conditions in the well by application of the equation of state for gas mixtures developed by Kunz et al. (2007). A vertical well discretisation with 100 elements was found to provide sufficient accuracy based on a sensitivity analysis. Pressure loss was determined to be <0.3 bar in the CO2 Ktzi 201/2007 injection well, and thus is neglected in the pressure correction calculations. The measured pressure at 550 m and the pressure corrected to 639.5 m depth (reference depth for reservoir simulations) as well as the cumulative injected CO_2 mass until the end of 2011 are shown in Fig. 5.

Results

Simulation of the pressure at reference depth in the CO2 Ktzi 201/2007 injection well as well as CO_2 arrival times in the observation wells CO2 Ktzi 200/2007 and CO2 Ktzi 202/2007 lead to results in good agreement with our observations applying permeability modifiers in two lateral areas of the reservoir model. For that purpose, a near-well area was defined for the range of $i = 30–64$ and $j = 49–79$ (origin in the upper left corner) and a far-well area for all elements not included in the near-well area considering the entire model thickness. Permeability multipliers were applied in both models to assign the revised permeabilities

in i-, j- and k-directions as listed in Table 1 to avoid an increase of simulated pressure not corresponding with the observations as of March 2010.

Table 2 shows the observed arrival times of gaseous CO_2 in both observation wells determined using a gas membrane sensor (Zimmer et al. 2011) as well as the simulated arrival times of gaseous and dissolved CO_2. In contrast to the results described by Kempka et al. (2010), the geological model is now able to provide a significantly better representation of the monitored CO_2 behaviour. This can be deduced from the agreement of simulated CO_2 arrival times at the CO2 Ktzi 200/2007 well with deviations of 6.4 % (ECLIPSE) and 11.1 % (TOUGH2) related to the observed data, as well as the match for the CO2 Ktzi 202/2007 well with deviations of 6.4 % (ECLIPSE) and 15.2 % (TOUGH2). Arrival times of dissolved CO_2 (not measured at the observation wells) are in agreement between both simulators for both observation wells.

The matching process was undertaken considering the pressure corrected to the reference depth in the CO2 Ktzi 201/2007 well and measured at 623.8 m in the CO2 Ktzi 202/2007 observation well (installed for about 1.5 years). The results illustrated in Fig. 6 show agreement at the CO2 Ktzi 201/2007 well for both simulators in the first 4 months of injection and a slight underestimation of pressure (by about 0.7 bars) by both simulators from month November 2008 to June 2009, whereas ECLIPSE results show a good

Table 1 Permeability multipliers applied at the near- and far-well areas as a result of the matching process for reservoir pressure and CO_2 arrival times

Permeability multiplier	Near-well area	Far-well area
i-direction	0.34	0.38
j-direction	0.07	0.10
k-direction	0.07	0.10

Table 2 Observed and simulated arrival times of gaseous and dissolved CO_2 in the observation wells CO2 Ktzi 200/2007 and CO2 Ktzi 202/2007

Observation well	Phase	Observed (days)	Simulated TOUGH2 (days)	Simulated ECLIPSE (days)	Deviation TOUGH2 (%)	Deviation ECLIPSE (%)
CO2 Ktzi 200/2007	Dissolved CO_2	–	10.6	11.0	–	–
	Gaseous CO_2	21.7	19.3	20.3	11.1	6.4
CO2 Ktzi 202/2007	Dissolved CO_2	–	221.4	225.0	–	–
	Gaseous CO_2	271	229.8	256.0	15.2	5.5
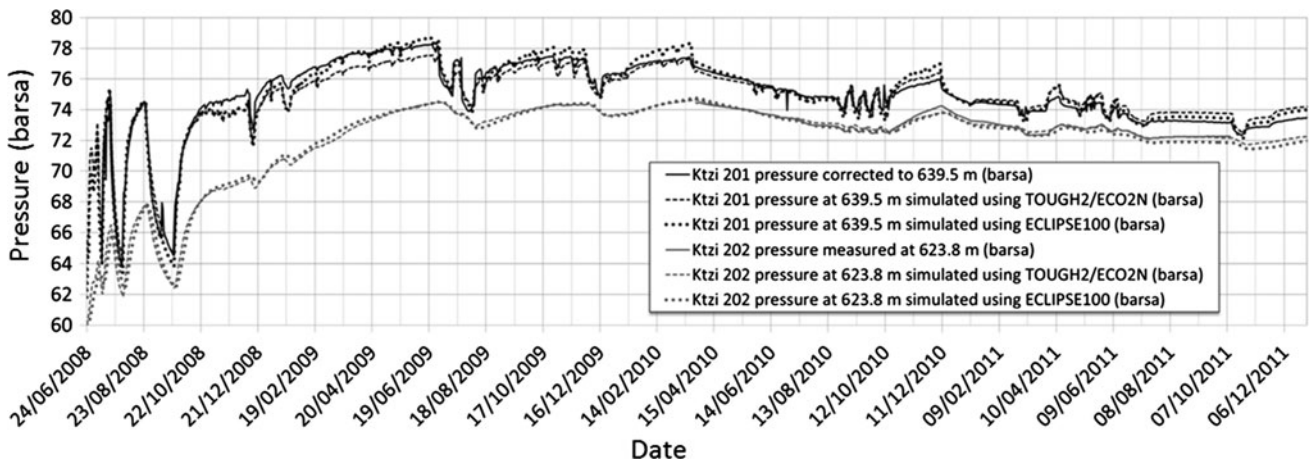
Fig. 6 Observed and matched pressure in the injection well CO2 Ktzi 201/2007 (permanent pressure monitoring) and the second observation well CO2 Ktzi 202/2007 (pressure sensor installed from May 2010 to October 2011)

match after February 2009. In the following months, the TOUGH2 results match with the observed data, while ECLIPSE tends to overestimate the pressure peaks resulting from injection at maximum rates (about 2.000 kg/s) by up to 0.8 bars. However, subsequently declining pressure is matched by the ECLIPSE simulator. Interference tests (alternating injection and shutdown) conducted from September to October 2010 are depicted by both simulators as well as different injection stops performed for monitoring campaigns and operational revisions during the entire timespan. The CO2 Ktzi 202/2007 pressure match is as well in agreement with the observations for both simulator results as well as for the comparison between both simulators against each other where monitoring data are not available (e.g. before May 2010).

Figure 7 shows the balance of injected, gaseous and dissolved CO_2 for the entire simulation time. Both simulation results are in agreement with each other. Peaks occurring in the ECLIPSE data are not present in the TOUGH2 data due to a limited amount of output data. However, the intermediate values coincide. Dissolution of CO_2 is slightly higher in the ECLIPSE model at the end of the simulated time.

Figure 8 shows CO_2 plume thickness isolines at 26 November 2008, 04 June 2009, 13 June 2010 and 31 July

2011. The simulations are in agreement at the first time steps with low deviations, e.g. the CO_2 plume calculated with TOUGH2 extends by 10–20 m earlier in northwest direction, while TOUGH2 results show a rather concentrated thickness around the injection well CO2 Ktzi 201/2007 for the two later time steps, whereby the overall CO_2 plume shape is almost identical. In general, maximum CO_2 plume thickness of up to 25.5 m is simulated at the CO2 Ktzi 201/2007 well and the lateral CO_2 plume size at the end of July 2011 is about $1,200 \times 1,000$ m. Figure 9 indicates that the saturation of the CO_2-rich phase calculated by both simulators at 31 July 2011 is almost identical with regard to shape and thickness. However, the well implementation in the TOUGH2 model leads to higher CO_2 saturations in the well elements compared to those calculated by ECLIPSE.

Discussion and conclusions

Within this manuscript, we outlined our most recent matching activities for the Ketzin pilot site based on a revised version of the initial static geological 3D model involving permeability fitting based on field observations of CO_2 arrival and pressure monitoring with its general
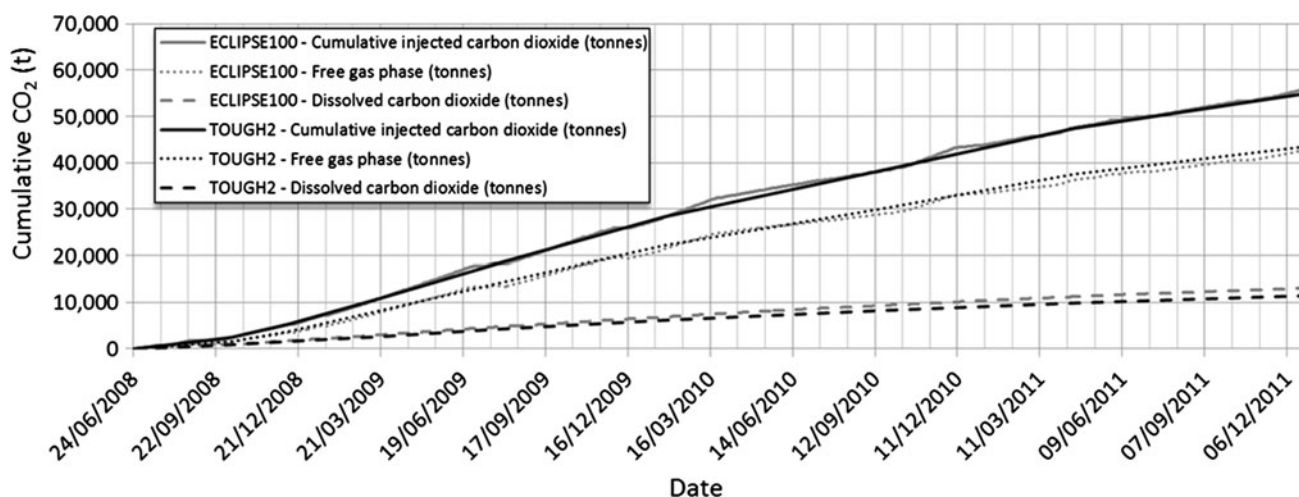
Fig. 7 Balance of total injected CO_2, free gas phase and dissolved CO_2 for both simulators applied

implementation discussed by Norden and Frykman (2013). For the numerical simulations we applied two different computer codes for comparison using a complex heterogeneous geological model taking into account all known reservoir properties: the industrial standard simulator ELCIPSE 100 and the scientific simulator TOUGH2-MP/ECO2N. A workflow for the conversion of complex Petrel models into TOUGH2 simulation models was developed and allows us now a fast integration of complex geometries like fault systems with offsets into the TOUGH2 simulator. Operational data of the Ketzin pilot site were integrated to parameterise the reservoir model.

Definition of a near- and far-field well area allowed us to assign different permeability modifiers in i-, j-, k-directions in order to achieve a successful match between observed and simulated data for the geological model (Table 1). A factor of about four in lateral anisotropy represented by the permeability multipliers which were determined during the matching process is in agreement with the hydraulic tests undertaken in advance of CO_2 injection in 2008 as discussed by Wiese et al. (2010).

Simulation results are in agreement with observed CO_2 arrival times, whereas TOUGH2 simulation results tend to have deviations of 11 % (CO2 Ktzi 200/2007) to 15 % (CO2 Ktzi 202/2007) compared to those of ECLIPSE with 5.5 % (CO2 Ktzi 202/2007) to 6.4 % (CO2 Ktzi 200/2007) as presented in Table 2. Considering the marginal variations of arrival time of dissolved CO_2 (Table 2) and the coincidence of CO_2 plume thickness and spatial extent over time (Fig. 8), we expect that the well implementation in the TOUGH2 reservoir model is responsible for the deviations encountered. Here, relatively high permeabilities of 1,000 mD were assigned to the well elements of 5 × 5 m lateral size leading to a decrease in the flow path by 5 m in total according to the double distance of the cell centre

(well location in ECLIPSE) to the element interface, as two well elements are always affected in this assessment. This explanation appears reasonable for both arrival times when considering, e.g. the CO_2 arrival at the CO2 Ktzi 202/2007 well with 258 days calculated by ECLIPSE and 229.8 days by TOUGH2, whereby an average flow velocity of 0.43 m/day is achieved. This would roughly sum up to about 240 days arrival time for the TOUGH2 simulation, even though the decrease of flow velocity due to the radial propagation of the CO_2 plume is neglected for this estimation.

The simulated pressure coincides with the reservoir pressure observed showing few deviations only. We expect that these are mainly caused by the different well implementations in both simulators. This assumption is underlined by the agreement of pressure data observed in the CO2 Ktzi 202/2007 well and the related pressures calculated by both simulators (Fig. 6).

CO_2 balance in terms of gaseous and dissolved CO_2 is comparable over the entire simulation time for both simulators (Fig. 7) and spatial distribution of the CO_2 plume and its thickness are also almost identical for both simulators (Fig. 8), whereby slight deviations (concentrated CO_2 plume thickness in the near-well area of CO2 Ktzi 201/2007 in the TOUGH2 results) are again expected to result from the different well implementations in both simulators. In the TOUGH2 model more CO_2 can be present in the CO2 Ktzi 201/2007 well elements due to the chosen porosity of 0.99.

Computational times of the TOUGH2-MP/ECO2N simulator were about 24 times higher for the current model compared to those of the ECLIPSE 2009.2 simulator using the same computer architecture. However, the application of a high performance computing cluster with 256 cores resulted in faster simulations compared to a sequential
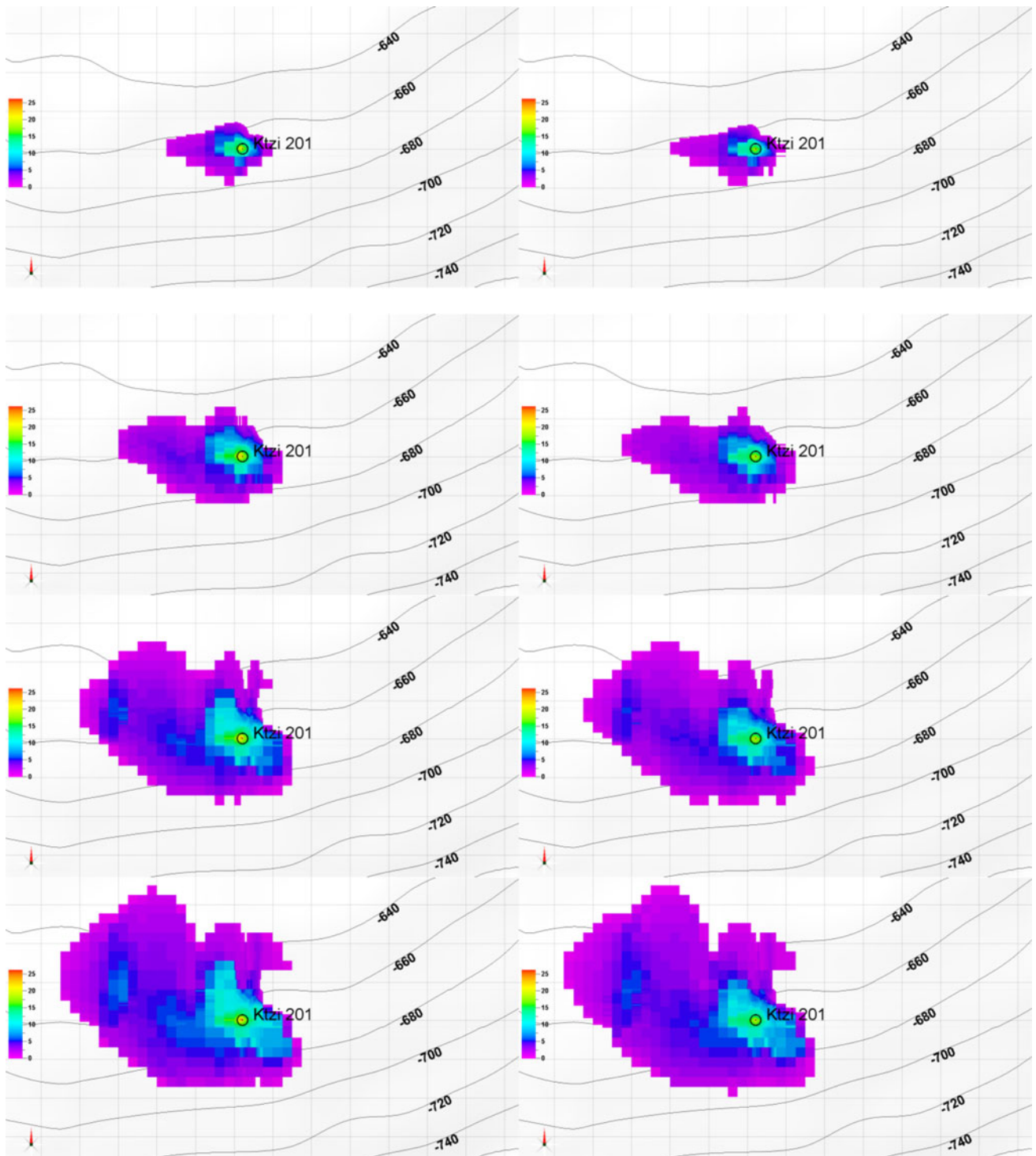
Fig. 8 CO$_2$ plume thickness in meter plots on 26 November 2008 (*first row*), 04 June 2009 (*second row*), 13 June 2010 (*third row*) and 31 July 2011 (*fourth row*), whereas ECLIPSE results are plotted *left* and TOUGH2 results *right*. The size of the *squares* in the background is 200 × 200 m

(single core) ECLIPSE run, where the total computational time was about 2 days.

In summary, we were able to achieve satisfying agreement between our simulation results with the world-wide unique monitoring data obtained at the Ketzin pilot site. We emphasize here that integration of all available operational and monitoring data improve the static geological model within the recurring update resulting in
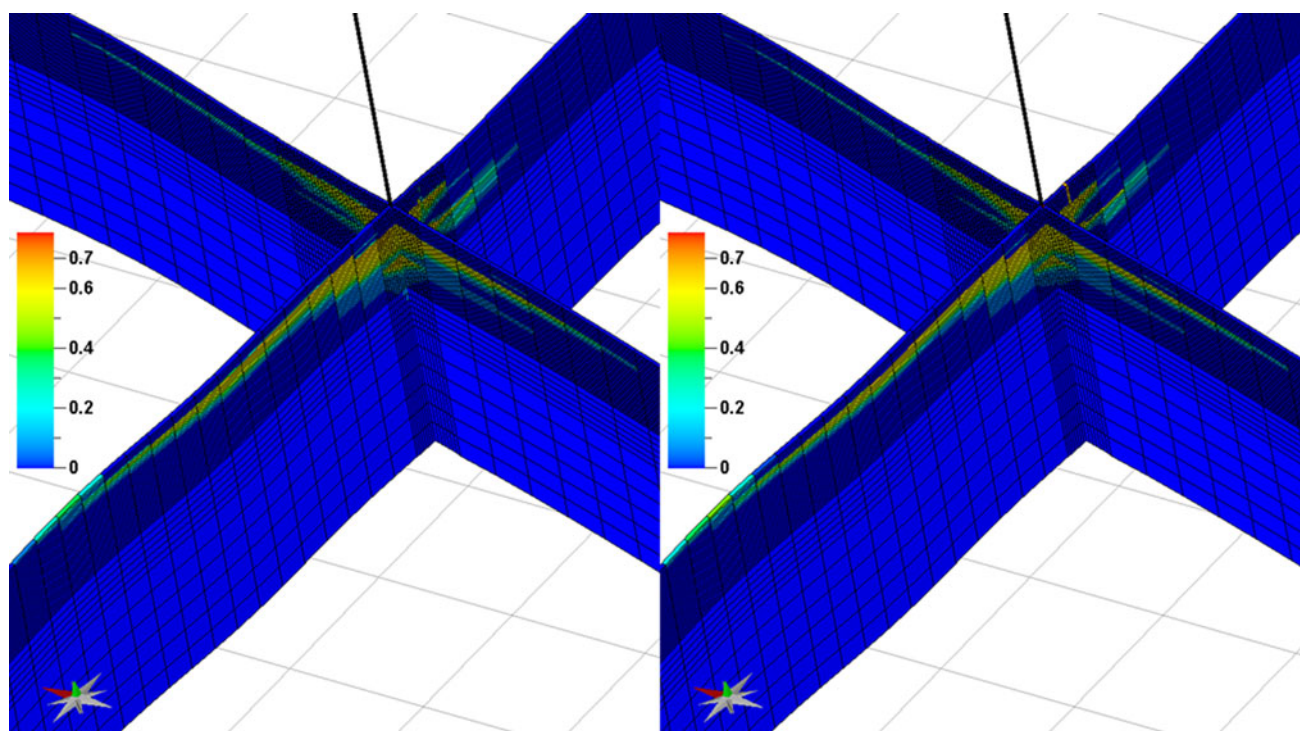
Fig. 9 Cross-section of the CO_2-rich phase saturation at the CO2 Ktzi 201/2007 injection well (indicated as *black line*) at 31 July 2011 calculated with ECLIPSE (*left*) and TOUGH2/ECO2N (*right*). Near-well lateral element size is 5 and 50 m thereafter, while element thickness in the uppermost zone corresponds to 0.5 m

better agreement with the measured data after each iteration round. This workflow provides us with a static model of advanced accuracy for further applications, for prediction of long-term site behaviour (e.g. pressure development and CO_2 migration) as well as guiding monitoring campaigns and site operation. Furthermore, we were able to demonstrate the applicability of industrial as well as scientific numerical simulators to successfully describe multi-phase flow processes in the Stuttgart Formation.

One of our next simulation tasks will be the prediction of the CO_2 plume shape and thickness for the upcoming 3D seismic repeat in fall 2012, whereby different modelling groups will be involved with their (in-house) simulation codes. Further activities will consider the enhancement of our Petrel-to-TOUGH2-MP workflow by local grid refinement (LGR, as available in Petrel and ECLIPSE) to allow for a realistic lateral well discretisation while maintaining the identical grid as applied in the ECLIPSE simulations. Implementation of data from core analysis from the CO2 Ktzi 203/2012 borehole (located in about 30 m distance of the CO2 Ktzi 201/2007 well on the connecting line to the CO2 Ktzi 202/2007 well) drilled in fall 2012 will allow further improvement of the static geological model in terms of facies-based heterogeneity development.

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