

# “CO<sub>2</sub>RINA”—CO<sub>2</sub> Storage Risk Integrated Analysis

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**Abstract** While risk assessment for CO<sub>2</sub>-storage often has been conducted by using a lot of simplifications and conservatisms, our approach developed in the CO<sub>2</sub>RINA-research project is based on the integration of all models, existing at a moment in time. These models will be coupled by the so called transfer function approach which has been proven to be very powerful in the risk assessment for low level radioactive waste. This concept ensures, that the risk assessment is always consistent with the state of the models existing for a specific site. It can be immediately improved if the existing models will be improved over time. The approach was verified by comparison of the direct coupling of different process models in an overall model with a coupling by transfer functions by conducting a wide range of test calculations showing very good accuracy of the approach. The new coupling approach allows the incorporation of a variety of additional effects which are difficult to handle in an overall model. Examples for such processes are complex chemical and microbiological interactions, geomechanical feedback loops and migration of CO<sub>2</sub> in the atmosphere. In the project there have been developed specified models for a generic site with parameters similar to the Ketzin site. These models

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include a reservoir model, a model for the alteration of the cementation of a mature well, a fault model, a model describing advection and diffusion through the cap rock, a complex model for the migration in a Quaternary aquifer including complex chemical interactions and a geomechanical model. Additionally there was shown the way of integration of microbiological processes which have been modelled in detail in the CO<sub>2</sub>BIOPERM project. The new approach is ready to be adapted to a specific CO<sub>2</sub>-storage site.

## 1 Background and Purpose

Risk assessment for CO<sub>2</sub> storage projects is mostly conducted using expert knowledge to evaluate specific scenarios. Features, events and processes (FEPs) are investigated to assess their impacts on operational and environmental safety. Oldenburg (2007) suggest an approach similar to a calculation sheet, whereas the interacting user defines relative parameter weight and processes as well as reliability of the available information by qualitative input and sorting methods. The drawback of such methods is the subjectivity related to decisions made by the interacting user. Oladyshkin et al. (2009) suggest the utilization of stochastic methods using a model reduction for specific scenarios to allow a reasonable application of Monte-Carlo simulations. However, efficient application of this method has to be verified for CO<sub>2</sub> storage projects acting at large spatial scales.

Numerical simulations are an established tool for prediction of thermal-hydraulic processes in geothermal reservoirs, oil and gas deposits as well as CO<sub>2</sub> storage formations at different time scales (Bielinski et al. 2008; Flemisch et al. 2007; Pruess and Spycher 2007; Pruess 2004; Pruess et al. 2003; Helmig 1997, u.v.a.) and were successfully applied within the scope of the EU-Project CO<sub>2</sub>SINK to provide reliable predictions for the CO<sub>2</sub> arrival in the observation well CO<sub>2</sub> Ktzi 200/2007 (Kempka et al. 2010a).

The thermal-hydraulic-mechanical simulations scheduled for prediction and evaluation of stress field changes in the vicinity of the storage reservoir were already successfully applied by parameterization and verification using InSAR data resulting from the CO<sub>2</sub> enhanced gas recovery (EGR) at the In Salah site in Algeria (Krechba gas field). The simulation results showed very good agreement between InSAR data and the time-specific modeling results of the coupled numerical tools for different areas in the near field of the injection wells of a storage formation located at about 1,800 m depth (Rutqvist et al. 2009a). Further studies conducted by Rutqvist and Tsang (2002), Rutqvist et al. (2002, 2007, 2008, 2009b), Wang et al. (2009), Watanabe et al. (2010), McDermott et al. (2010), Nowak et al. (2010) and Park et al. (2010) demonstrate the suitability of the coupled numerical models intended for application with the proposed project to determine stress field changes in a CO<sub>2</sub> storage formation to predict and evaluate failure criteria of relevant parameters in the storage formation and its cap rocks as well as potentials for reactivation of faults.

It can be concluded that the extensive national and international efforts in the research field of CO<sub>2</sub> storage in geological formations provided a basic conceptual understanding of the relevant processes in the CO<sub>2</sub> storage formation as well as the different migration pathways into the overburden and surrounding rocks (CSLF-T 2009; Deel 2007; Metz et al. 2005; Walton 2005; Nordbotten et al. 2005; DOE 2009). Currently, these processes can be reliably described assuming well-known geological boundary conditions and input parameters (Zhang et al. 2006; Zhou et al. 2005; Celia et al. 2005).

Very different approaches exist to integrate the specific processes relevant for the risk assessment of long-term geological storage of CO<sub>2</sub> (Jagger 2009; Espie 2005; Cugini et al. 2010; Saripalli et al. 2003; Wildenborg et al. 2005; Pawar et al. 2006; Condor and Unatrakarn 2010). Suggested methodologies integrate approaches such as systematic cause and effect analysis (SWIFT) and Monte-Carlo based methods (RISQUE). In addition, methods based on evidence (TESLA) not considering the classic Boolean logic, but taking into account that an assumption may be wrong, correct or even involve an uncertainty. The evidence based method was originally developed for application in nuclear waste storage. Further approaches for risk assessment of CO<sub>2</sub> storage projects were derived from the evaluation of nuclear waste storage sites (North 1999). Regarding nuclear waste storage, the methods for risk assessment were extensively addressed by Ho (1992) and North (1999) and updated by Maul et al. (2007).

Within the scope of the proposed study we aim to implement and apply an approach comparable to those developed for nuclear waste storage considering its methodology (Stauffer et al. 2005, 2006, 2007, 2009; Viswanathan et al. 2005, 2008). However, the targeted approach strongly deviates in the implementation of the model coupling required for the overall risk assessment. The simulation tool intended to be applied to couple the specific process models will be the GoldSim software package as already addressed by Stauffer et al. (2007) within the scope of the CO<sub>2</sub>-PENS methodology. This probabilistic simulation tool was originally developed for the assessment of the Yucca Mountain nuclear waste storage site and provides high flexibility regarding the simulation of arbitrary and highly dynamic systems. Kahnt (2006, 2008), Kahnt and Paul (2008) developed a methodology for the assessment of longterm storage of low radioactive waste materials based on the GoldSim software package (CSM-Approach). The CSM-Approach is based on the coupling of different dynamical processes. While process models such as FEHM (Zyvoloski et al. 1997) and TOUGH2 (Zhang et al. 2006) as well as (semi-) analytical methods (Nordbotten et al. 2005) are directly operated by the GoldSim software package in the CO<sub>2</sub>-PENS project, the CSM-Approach provides generic flexible interfaces. Thus, arbitrary process models can be exchanged and extended independently. These flexible interfaces have been used for coupling the Box Model (Module C) applied for coupled 3D-simulations of geochemical processes to the GoldSim system simulation model (Kahnt 2006, 2008; Kahnt and Paul 2008).

The main goal of the conducted work was the adaptation of the risk assessment methodology developed for low level radioactive waste for the risk assessment of CO<sub>2</sub> storage in geological media, its numerical realization and specific validation

based on data from natural analogue studies and a present CO<sub>2</sub> storage pilot site. The newly developed methodology is mainly based on the international risk assessment concepts described before.

For this purpose, the geological system involving its technical elements is simulated over a specific timespan in order to assess the probability of CO<sub>2</sub> release with regard to spatial and temporal parameter dependence.

The challenge of risk assessment is the fact that different processes and their combinations influence CO<sub>2</sub> migration into shallow geological formations or the atmosphere. Here, conceptual uncertainties (which processes will dominate?) as well as parameter uncertainties (specific process parameters and their variability cannot be exactly determined due to geological heterogeneities) and parameter variability have to be considered. Even though a deterministic methodology is required for the assessment of the multiple specific processes and their interaction, a probabilistic approach has to be applied at the cross-system level to represent parameter variability and parameter uncertainties in the quality required for risk assessment.

To allow for high transparency for the evaluation and selection of potential storage sites as well as decision support system tools for regulatory authorities, a common and site-unspecific methodology flexible enough to be adapted to any specific site location was developed.

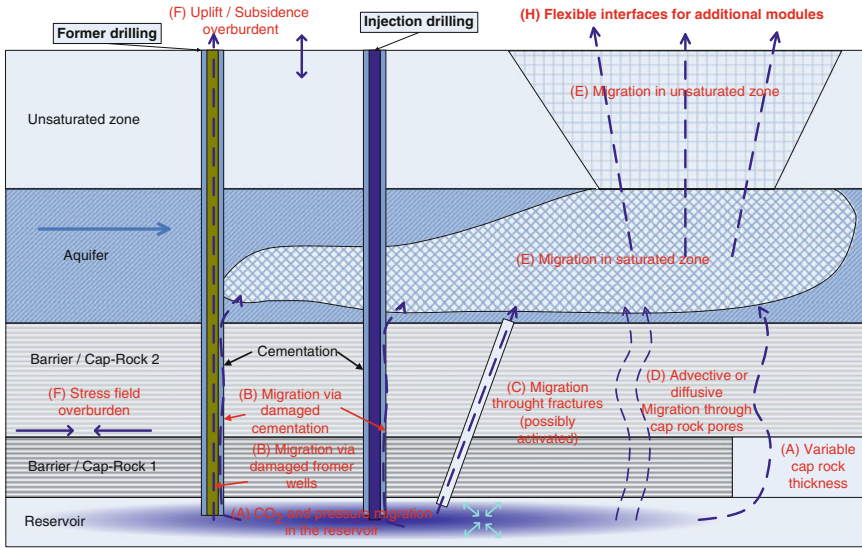
The developed approach provides an improved methodology in comparison to the tools available on the international market, since it is set up consequently modular taking into account clearly defined interfaces. By this, existing site-specific models can be consistently implemented into the risk assessment model and coupled with each other. The single modules can be further developed independently and be flexibly exchanged.

The methodological solution is based on segmentation of multiple coupled general problem simulation into single defined problem simulation modules. Communicating via expert interfaces a combination of sub-solutions from these single modules can be integrated to solve the main problem module simulation.

An general overview of the integration of the different modules is given in Fig. 1.

Before the description of single modules is presented in detail, major aspects of the procedure will be explained here to ensure the understanding of their relevance in the overall solution approach:

- The project targets the development of a consistent methodology for risk assessment based on modular description of a main system. At the core of this work the method of probabilistic modelling and associated correlation analysis allows the identification of processes and parameters regarding their site-specific contribution strength to the overall risk, which is an essential step to optimize objectivity in the assessment process. Processes and parameters from different fields of work are further investigated regarding the influence of potential cross-communicating sub-processes by directly simulating the influence of diverse counteractive measures on different single units and the main system itself.



**Fig. 1** Schematic overview about CO<sub>2</sub>-release pathways and related single processes covered by the different modules (for processes red text was used, while for structures black text has been used). The letters A–H have been used for the enumeration of the different modules

This vice versa allows the assessment of effectivity and quality of each counteractive measure to reduce the overall risk. In a possible additional step the costs of the different counteractive measures can be compared to the effectivity (quality) factor of each counteractive measure, giving the basis for optimized risk assessment solutions. The methodology thus directly reclines to the concept of specific site conditions that has been developed for clean up decisions in the field of low radioactive mining wastes.

- The identification of applicable interfaces between the single modules is of major importance. The basic target behind this approach is the idea to guarantee the possibility of single module replacement. Following this idea, different conceptual approaches as well as different software tools are applicable for the sub-processes simultaneously without communication conflicts. A main focus was kept on the possibility to further develop the single modules independently.
- In order to demonstrate the applicability of the solution approach it was necessary to test real problem scenarios and use site-specific data streams. This has been done using generic data from the EC funded project CO<sub>2</sub>SINK at the Ketzin-site together with associated modelling tools to verify the applicability of the single modules. An important aspect of the concept-verification is the possibility to resort to much more quantitative and qualitative data at the Ketzin-site, as in comparison to theoretical validation.
- Besides the development of probabilistic risk solutions, the solutions themselves have been validated for several sub processes using deterministic approaches.

In this context the coupling was verified not only in modules with defined interfaces but as well in deterministic models to verify the probabilistic approaches.

- The methodology of risk analysis was developed on a general basis, allowing to consider site specific geological conditions as well as potential pre-existent site specific models and calculation tools.

## 2 Module Description

### 2.1 Module (0) System Simulation Model Development

The different modules of the project have been illustrated in Fig. 1. Module (0) represents the main system simulation model in which all residual modules can be integrated in. For that integration, the software GoldSim was used. This software type has been developed with key focus on risk analyses. Subsequently the basic conceptual idea of the main system simulation model is presented.

Each single module consists of either partly already available and/or new methodologies which have been developed for the sub-processes. Using the complete spectrum of these methodologies the interrelationship between module input parameters and target functions can be calculated. Using various simulation scenarios the total number of target functions in dependency of sensitive module input parameters will be determined. The resulting interrelationship data sets will be stored in multidimensional look-up-tables. These tables are used in the main system simulation model in order to consider all interrelationships of underlying single processes. One of the key challenges was to figure out the interface parameters and the types of interfaces/look up tables.

Within the main system simulations model all single processes are interconnected in a way that, all former single parameter dependencies among each other are maintained. The total spectrum of key parameters is determined together with the related uncertainties and integrated into the main system simulation model by using distribution functions.

Resorting to Monte-Carlo simulations the influence of parameter uncertainties on target parameters was determined. The target parameters of each module as well as the interface between the modules have been specified.

Due to the legal foundations, CO<sub>2</sub> storage operations have to consider the risks for the subjects of protection air, water and soil. Especially there have been calculated concentrations of CO<sub>2</sub> and other species at different points in the geosphere as well as mass fluxes. Additionally geomechanical deformations have been evaluated.

The main simulation model was developed under consideration and awareness of the possibility to be adapted to different site-specific conditions.

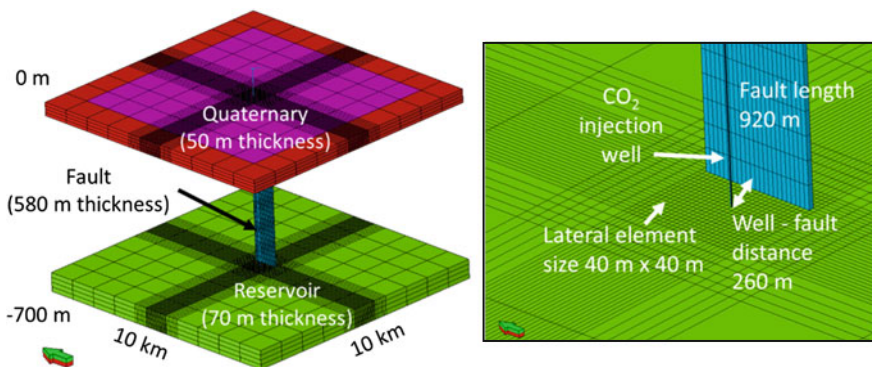
The presented solution approach offers the possibility to identify the parameter uncertainties with greatest effect on target parameters using sensitivity analyses. Subsequent investigations can thus be focussed on the resulting key parameters. Operating this way, the procedure enforces the reduction of investigation demand and resulting costs. The structure of the methodological solution into single modules reflecting the process chain is shown in Fig. 1.

The single modules are interconnected via multi-dimensional look-up tables, delivering input–output inter-relationships. The definition of appropriate input and output modes was a major challenge for the development of the methodology, because the coupling has to ensure consistency.

### 2.2 Module (A): Reservoir Simulations/Numerical System Simulation Model

A 3D numerical system simulation model including the CO<sub>2</sub> storage reservoir, the hydraulically conductive fault and the shallow aquifer has been implemented to serve as reference and for verification of the process and model coupling approaches. Numerical simulation results such as pore pressure and mass flow across specific interfaces serve as main input for the GoldSim system model in module 0, and thus for all models coupled to it. Figure 2 shows the employed generic numerical model grid with an areal extent of 10 km × 10 km and a total thickness of 700 m. Three main areas are distinguished: the reservoir being used for CO<sub>2</sub> injection, the leaky fault and the shallow Quaternary groundwater aquifer.

Applied generic porosities and permeabilities are listed in Table 1, while relative permeabilities were derived from Kempka et al. (2010) and Kempka and Kühn



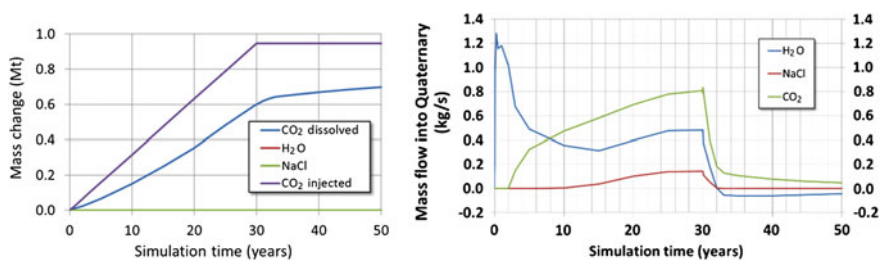
**Fig. 2** Left numerical system simulation model including the reservoir (green), the fault (light blue) and the quaternary (magenta and red). Right close-up view of the injection and fault area in the numerical system simulation model indicating the local grid discretization in the reservoir (green) and at the fault (light blue)

**Table 1** Porosity and permeability applied in the numerical system simulation model

Model unit	Porosity (%)	Permeability in x- and y-direction (m <sup>2</sup> )	Permeability in z-direction (m <sup>2</sup> )
Quaternary	25	10 <sup>-10</sup>	3.33 <sup>-10</sup>
Reservoir	25	10 <sup>-13</sup>	3.33 <sup>-13</sup>
Fault	1	10 <sup>-12</sup>	10 <sup>-12</sup>

(2013). Reservoir salinity is set to 25 % by weight (Klein et al. 2013) to represent realistic conditions for density, Quaternary salinity is zero. This density difference has major impacts on reservoir pressure which is required for brine flux through the fault. 1 kg CO<sub>2</sub>/s is injected for 30 years via the injection well plotted in Fig. 3 (left) resulting in a total injected CO<sub>2</sub> mass of about 0.95 Mt at the end of the simulation. A post-injection phase of 20 years is applied thereafter, so that the total simulation time amounts to 50 years. The numerical simulator TOUGH-MP/ECO<sub>2</sub>N (Pruess 2005a, b; Zhang et al. 2008) was applied for the simulation.

Simulation results indicate that about 73 % of the injected CO<sub>2</sub> have been dissolved in the formation fluid until the end of the simulation time (50 years) as plotted in Fig. 3 (left). As expected, CO<sub>2</sub> dissolution is proceeding even after the injection stop at 30 years of simulation. Figure 3 (right) illustrates that CO<sub>2</sub> and brine arrive after about 2 years of injection in the shallow Quaternary aquifer, while water (no mineralization) being present in the residual fault pore volume is migrating into the Quaternary aquifer from the beginning of CO<sub>2</sub> injection. With the CO<sub>2</sub> arrival in the Quaternary aquifer (after about 2 years) the H<sub>2</sub>O mass flow through the fault decreases until the saline formation fluid arrives at the Quaternary aquifer in simulation year 9. This is caused by the increasing density in the fault. Thereafter, CO<sub>2</sub>, H<sub>2</sub>O and NaCl displacement into the Quaternary aquifer increases to a maximum until the stop of injection in year 30. From then on, a significant reduction of CO<sub>2</sub> and NaCl as well as H<sub>2</sub>O flux rates can be observed. H<sub>2</sub>O starts to flow back into the fault and reservoir after year 32 at a low rate of about 0.05 kg/s. In total, about 65 % of the injected CO<sub>2</sub> is displaced into the Quaternary accompanied by 0.7 Mt NaCl originating from the reservoir. Hereby, the maximum reservoir pressure elevation amounts to about 1.4 MPa at the injection well top. The



**Fig. 3** Left numerical system model mass balance change during the entire simulation time of 50 years. Right component mass flow of CO<sub>2</sub>, H<sub>2</sub>O and NaCl into the shallow quaternary aquifer



huge part of CO<sub>2</sub> displaced into the Quaternary is caused by the boundary conditions of the system which have been chosen such, that during the simulation time significant leakage effects will show up.

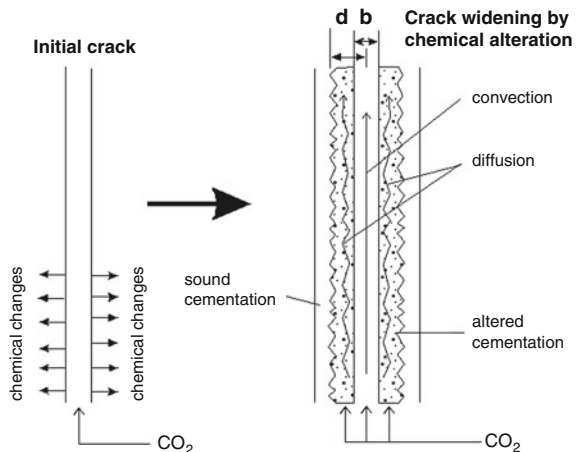
The introduced reference model with the given parameterization is employed in a simulation framework that allows for automated massive parallel simulations. Consequently, Monte-Carlo simulations were applied to validate the system model based on the GoldSim software package based on varying parameter realizations. Furthermore, the coupled process simulations were implemented for a specific validation of hydro-mechanical processes related to effective stress dependent fault aperture as a function of pore pressure.

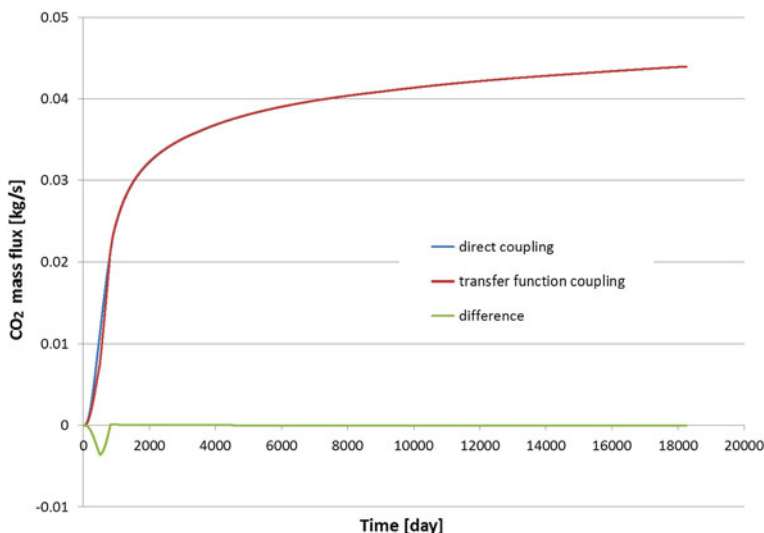
### 2.3 Module (B): Migration Through an Abandoned Well

The model for an abandoned well was initially developed in a separate GoldSim™ model. In this model there is described the transient development of the degradation of the cementation of the well and the resulting widening of an initially existing micro fracture. The basic conceptual model is shown in Fig. 4.

Because of that, the module (B) could be used for initial benchmark calculations of the overall coupling concept, because the GoldSim model can be used separately and the effects can be incorporated as transfer functions/look up tables on the one hand side and the model can be incorporated into the overall GoldSim model directly. By comparison of the results of both modelling concepts, the coupling approach was verified. The comparison is shown for one example calculation in Fig. 5. The result demonstrates that the transfer function coupling approach seems to work very well.

**Fig. 4** Conceptual model for the chemical widening of an initial microfracture in the cementation  $b$  is the opening of the fracture and  $d$  is the carbonization depth





**Fig. 5** Comparison of the CO<sub>2</sub>-mass flux through the cementation of an abandoned well calculated by direct model coupling and alternatively by transfer functions according to module (B). The *green curve* is the difference between the two calculations

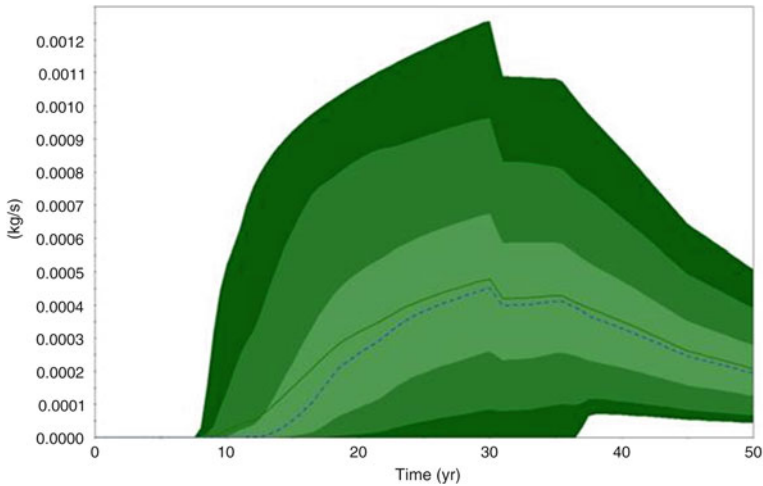
Using this model for the abandoned well coupled with the reservoir model, there has been calculated the probability distribution of the CO<sub>2</sub> mass flux through the well as a function of time taking into account all parameter uncertainties. The result is shown in Fig. 6.

#### **2.4 Module (C): Migration Through Fractured Zones**

Faults and fractured zones are of major importance for a safe long-term storage as they may hydraulically connect various geological units. The width of the fault/fractured zone and its permeability are determining factors for the CO<sub>2</sub>-storage. Faults can show high permeabilities but they can also act as flow barriers. Changing the stress conditions by injecting CO<sub>2</sub> and, thus, increasing the pore pressure can reactivate previously inactive zones of weakness. Chemical reactions between CO<sub>2</sub> and minerals of the host rock or of precipitated minerals in the fault zone can have an influence on the permeability—both positive and negative.

In geological time frames, induced natural geomechanical processes may lead to a fracturing of the cap rock or a reactivation of fault zones associated with an increase in permeability. Here, an increased swelling capacity of the cap rock will be of particular advantage for the tightness of the storage complex.

In the model used here with a thickness of the cap rock barrier of 120 m with a displacement of only 20–30 m, a sealing effect is likely to occur. Based on diagrams



**Fig. 6** Distribution function for the time dependent CO<sub>2</sub> mass flux through the cementation of an abandoned well taking into account different parameter uncertainties, like initial opening of the fracture, reaction rate and initial transmissivity of the fracture. The *dotted blue line* is the average value, the *green line* is the median and the different green areas give the percentiles (5, 10, 25, 75, 90 and 95 %)

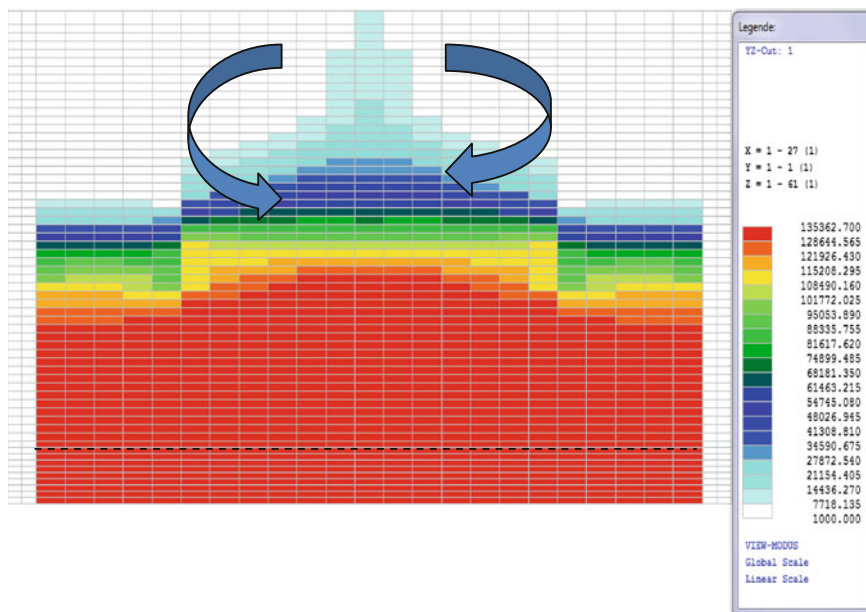
showing typical ratios the width of the (typically tight) fault core should amount to a maximum of 3 m, the (more permeable) damage zone up to 100 m. It has to be noted, however, that the values can vary in the range of two orders of magnitude!

The modeling in the CO<sub>2</sub>RINA-frame-project is concentrated to these fault zones, especially to consider following processes:

- Turbulent flow considering variable gradients with rough-laminar, rough-turbulent, smooth-laminar, smooth-turbulent flow conditions
- Time depended fracture width (coupled with an geomechanical model)
- Two phase flow CO<sub>2</sub>-H<sub>2</sub>O
- Reactive multi-migrant-transport with precipitation and dissolution of minerals in the fault
- Density driven flow

In the first step the 2-phase-flow was adapted into Reacflow3D (an existing multi-migrant-model) according to the concept of the “fractional flow formulation” [Niessner] and thoroughly tested in comparison with the modeling systems [MUFTE-UG] and [Dumux]. Furthermore some plausibility checks carried out, especially for the control of the density effects in comparison with the modeling system. [Tough2].

After developing an interface for transferring time depending fractures-widths and implement turbulent flow laws, the hydraulic situation in the fault was investigated with the help of the expanded model.

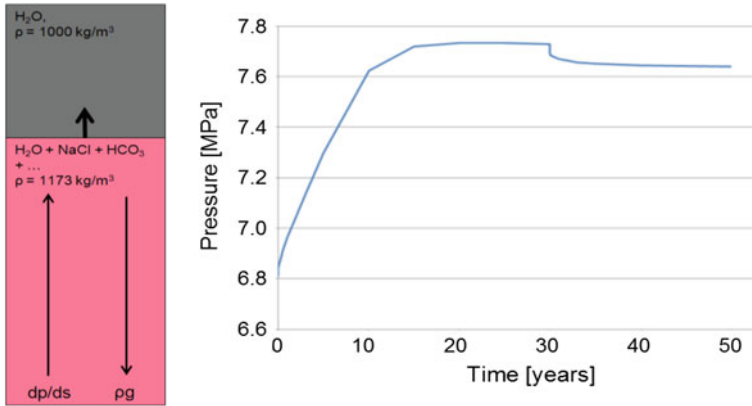


**Fig. 7** Distribution of chloride concentration in the fault zone (concentration on a *vertical* plane inside the fault zone) 2 years after start of  $\text{CO}_2$ -injection in the reservoir. *Red colors* indicate concentration of about 135 g/l representing the initial concentration of the reservoir brine, while the concentration on *top* of the fault has been diluted (see concentration legend). The reservoir below the fault zone is represented by the lowest 8 grid rows (below *dotted black line*) while the quaternary aquifer is located above the *uppermost* grid row

Apart of the new developments in Reacflow3D the emphasis is the investigation, how several types of models (injection zone, fault, groundwater and geochemistry) can interact with each other to get a joint result. It is known from series of real examples that the models of several hydraulic horizons are becoming increasingly complex, so that the overall model is limited in the numbers of considered processes or by the calculation time. As a result a proper coupling procedure is necessary. This means: “decoupling of the complex problem”.

Figure 7 gives an impression about the complex flow process in the fault zone caused by density effects. In the middle part of the fault zone in a short rectangular distance to the injection point, the chloride-front is reaching after nearly 10 years the upper quaternary groundwater layer. A few meters away the pressure in the injection horizon is not high enough to lift the heavy salt-column up to the groundwater layer. A circulation of salt water occurs from the middle column to the sides. It illustrates the sensitivity of the flow field caused by density effects.

Figure 8 simplifies this problem into one dimension. The pressure gradient is approximately in (very sensitive) equilibrium with the gravity and the pressure in the injections horizon is increasing up to the level, where the salt water is raising to the quaternary horizon:



**Fig. 8** *Left* force balance between gravity term and pressure gradient. *Right* temporal development of the pressure at the *bottom* of the fault for the central element of below the fault

The original concept to couple the model of the injection horizon with the fault model by transfer of the boundary-variables “pressure” and “CO<sub>2</sub>-Saturation” failed, because little differences in some model internal formulas (e.g. density-concentration) led to very big differences in flux of CO<sub>2</sub>-gas and raising salt water flow, although in principle all models worked correct.

The consequence of this effect was that the fault zone has to be incorporated into the reservoir model as a boundary condition to maintain an exact overall mass-balance. Additional processes of higher order can be incorporated separately.

From this point of view there was developed a concept, where the Reactflow3D-Model is modeling the change of hydraulic condition by different effects, e.g. fracture width, chemical reactions, and the results were transferred to GoldSim.

GoldSim assigns the different variants with the overall mass balance using the mass-flow of salt water and the hydraulic gradient.

### 2.5 Modul (D): Advective and Diffusive Flux Through the Cap Rock

Two processes have to be taken into account when considering the safe and long-term sealing capacity of an intact and water-saturated seal (cap rock) that is in direct contact with the free CO<sub>2</sub> phase of the storage layer: (1) Capillary pressure-controlled viscous flow of CO<sub>2</sub> through the seal and (2) molecular diffusion of CO<sub>2</sub> dissolved in the pore water of the cap rock.

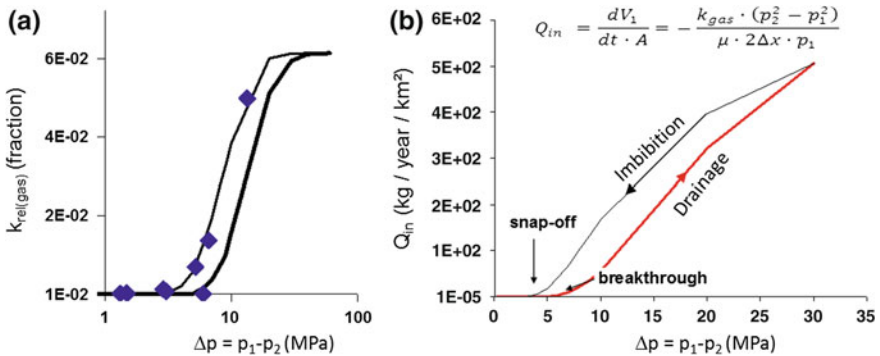
The first process depends on the critical capillary threshold pressure ( $p_{brthr}$ ), which must be overcome for CO<sub>2</sub> to displace the water and enter the interconnected pore system of the cap rock. Whenever this pressure is exceeded viscous flow of CO<sub>2</sub> into the cap rock will occur which can lead to a leakage flow in the long term.

In the *worst-case scenario* of capillary gas breakthrough the water saturation of the cap rock pore system successively decreases with increasing CO<sub>2</sub> (capillary) pressure, i.e. the pressure difference between gas (p<sub>1</sub>) and water phase (p<sub>2</sub>). In consequence the conductivity for the gas phase increases, leading to increasing leakage rates (Q). Successive depletion of the CO<sub>2</sub> accumulation leads to a reduction of gas pressure and the (reverse) process of water re-imbibition into the cap rock pores. This will reduce the relative gas permeability ( $k_{rel(gas)} = k_{gas}/k_{intrinsic}$ ) until the pore system is completely blocked by the water phase when the capillary snap-off pressure is reached. This pressure is somewhat lower than the initial breakthrough pressure ( $p_{brthr} > p_{snap-off}$ ) (Busch and Amann-Hildenbrand 2013). Due to this phenomenon capillary sealing would become effective again and CO<sub>2</sub> leakage from the reservoir would stop (Hildenbrand et al. 2003, 2004).

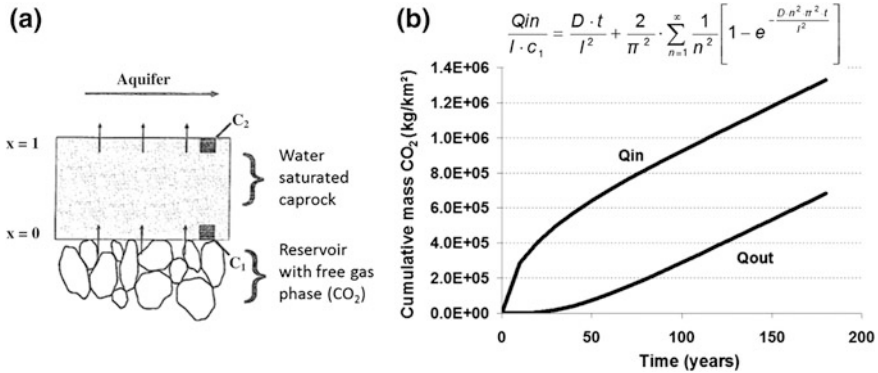
The gas leakage rate after capillary breakthrough can be quantified as function of the capillary pressure. Based on measured capillary pressure versus relative gas permeability data (Amann-Hildenbrand et al. 2013) and assuming a log-normal pore size distribution we have estimated the leakage rates from a CO<sub>2</sub> reservoir using Darcy’s law for compressible media (Fig. 9).

In contrast to capillary controlled transport, diffusion is considered a continuous and ubiquitous process with low transport capacity. At the reservoir/cap rock interface CO<sub>2</sub> will dissolve in and equilibrate with the pore water. The dissolved CO<sub>2</sub> will diffuse upward, following the concentration (chemical potential) gradient. This process is described by Fick’s laws of diffusion (Crank 1975).

The process is approximated by assuming diffusion through a homogeneous plane sheet (cap rock) of given thickness (x = l) (Crank 1975; Krooss et al. 1992a, b; Schlömer 1998). The bulk CO<sub>2</sub> concentration at the *base* of the cap rock ( $c_1 = c_{pore\ water} \cdot \phi$ ) is a function of temperature, pressure and salinity (Duan and Sun 2003) and porosity. Because the variations are small this concentration is assumed constant throughout the process. The concentration at the *top* of the cap rock (c<sub>2</sub>) is assumed



**Fig. 9** a Relative gas permeability as function of capillary pressure based on data from Amann-Hildenbrand et al. (2013). b Leakage rate out of the reservoir into the sealing lithology (Q<sub>in</sub>) by immiscible viscous gas flow



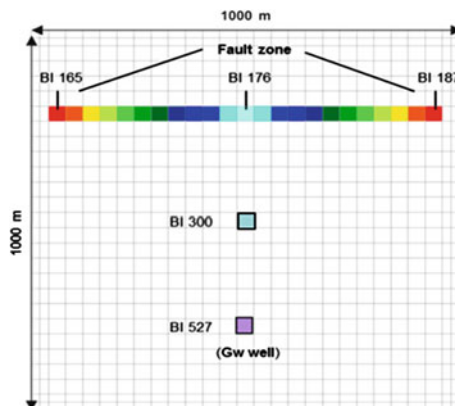
**Fig. 10** **a** Basic model for diffusion through a cap rock with thickness  $l$ ,  $c_1$  the concentration on the reservoir/cap rock interface and  $c^2$  at the top of the cap rock sequence ( $c^2 = 0 = \text{const.}$ ) (Schlömer 1998). **b** Cumulative mass of CO<sub>2</sub> diffused into ( $Q_{in}$ ) and out of ( $Q_{out}$ ) 1 m<sup>2</sup> of a cap rock layer of 160 m thickness

to be constantly zero. Figure 10 shows the calculated cumulative masses of CO<sub>2</sub> entering (at the bottom) and leaving (at the top) one square metre of a 160 m thick cap rock layer as a function of time. Input parameters were:  $l = 160$  m,  $\phi = 12\%$ ,  $T = 34$  °C,  $p_1 = 6.3$  MPa, salinity 1.1 mol NaCl/kg water. The effective diffusion coefficient assumed for this calculation ( $5 \times 10^{-10}$  m<sup>2</sup>/s) is at the upper boundary of values reported in literature, ranging from  $10^{-10}$  to  $10^{-12}$  m<sup>2</sup>/s for shales, clays and carbonates (Busch et al. 2008; Song and Zhang 2013).

The contribution of the described processes to the overall CO<sub>2</sub>-leakage risk has been assessed extensively. These processes only contribute in the long term, i.e. on time scales of some thousand years to the leakage and therefore can be neglected if processes during the injection phase become dominant in their risk contribution. This approach is the consequence of the top-down approach underlying the whole CO<sub>2</sub>RINA concept.

### 2.6 Module (E): Fluid Migration in the Unsaturated and Saturated Zone

Quantified prognoses for atmospheric CO<sub>2</sub> outgassing via the unsaturated zone and accompanied groundwater chemistry changes like acidification and salinization are key challenges for reliable integrated long-term CO<sub>2</sub> storage risk assessment tools. In view of numerical solutions a first starting point may thus be set to CO<sub>2</sub> phase partitioning behaviour between liquid and gas phase within the saturated zone. Referring to exemplary brine and groundwater chemistry data sets near the Ketzin pilot site (e.g. LUA 2007; Seis et al. 2013) in this context currently various scenarios are analysed using the software code boxmodel ReacFlow3D (Eckart 2011).



**Fig. 11** Model aquifer (*top view*) with different observation points (BI) at which the concentration histories have been evaluated. The different observation points are marked with different colours. Same colours have been used for symmetric points which show the same concentrations

With regard to the schematic conceptual overview and main aquifer boundary conditions in Fig. 11 and Table 2, Figs. 12, 13, 14 and 15 provide first rough long-time saturated zone snapshots of expected CO<sub>2</sub> liquid/gas phase partitioning, chloride- as well as related density-levels, assuming a leaking reservoir brine at a mass flow rate of 1 kg/s with a CO<sub>2</sub>/H<sub>2</sub>O mass-ratio of 0.08.

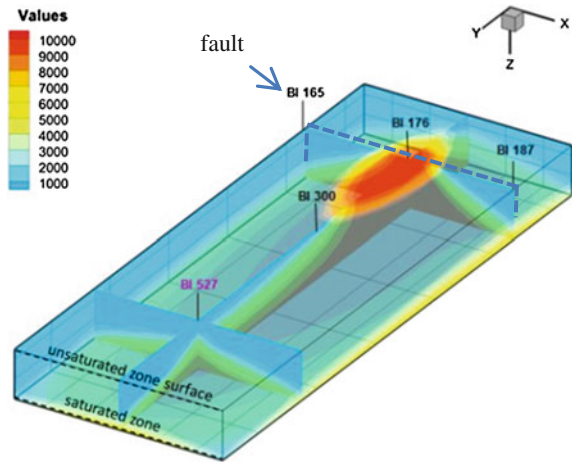
With focus on main trends under the selected boundary conditions seen so far commonly >90 % of CO<sub>2</sub> remains dissolved in the liquid phase and only marginal amounts are available in the gas phase for atmospheric outgassing (cf. Figs. 12 and 13). CO<sub>2</sub> liquid phase transport is merely controlled by density changes related to variable brine chemistry Cl<sup>-</sup> levels, as seen in quite similar spatial distributions. Simultaneously many scenarios indicate Cl<sup>-</sup> is likely to exceed the drinking water limit of 250 mg/l.

**Table 2** Aquifer boundary conditions

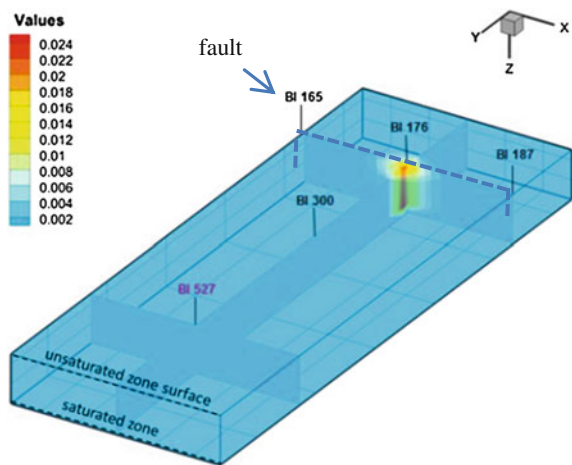
Length × width × height	(m)	1,000 × 1,000 × 50
h-potential well BI 527	(m)	25
h-potential residual aquifer	(m)	30
Bottom level well BI 527	(m)	-16
Start up groundwater background levels at t = 0		
CO <sub>2</sub> dissolved liquid phase	(mg/l)	290
CO <sub>2</sub> gas phase	(kg/s)	0
Cl <sup>-</sup> dissolved liquid phase	(mg/l)	70
Density	(kg/m <sup>3</sup> )	1,000



**Fig. 12** CO<sub>2</sub> dissolved in aqueous phase (mg/l) distribution after t = 50a



**Fig. 13** CO<sub>2</sub> gas phase flux rate (kg/s) distribution after t = 50a

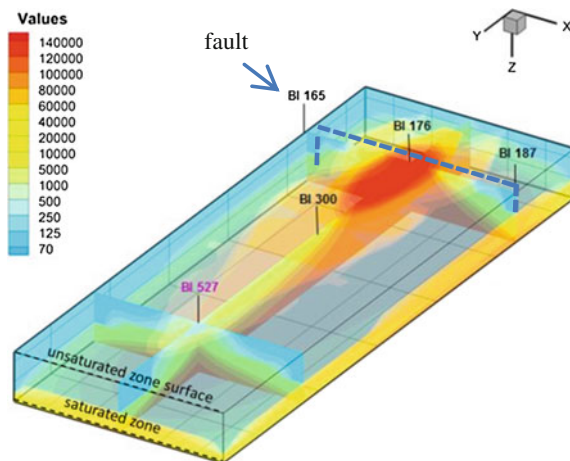


Within the aquifer overall minor mixed fluid phase upward migration is observed, in accordance with higher brine related density levels (cf. Figs. 14 and 15).

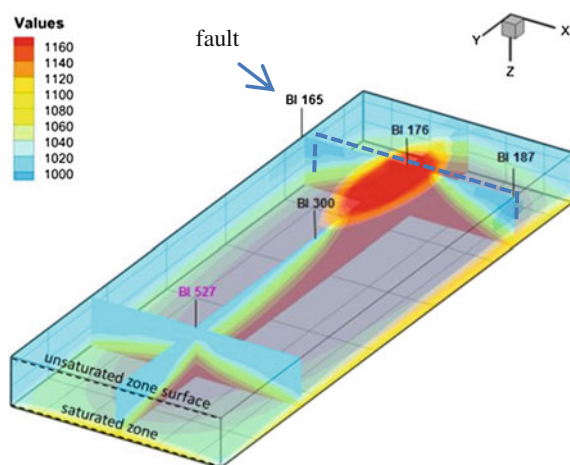
### 2.7 Module (F): Geomechanical Modelling of Stress/Strain State of the Cap Rock and Reactivation of Fault Zones

Module F deals with the geomechanical modelling of an onshore CO<sub>2</sub> storage site. For this the cap rock integrity, the deformation of the ground surface and the hydraulic reactivation of existing fault zones are investigated. Based on the synthetic model of the CO<sub>2</sub>RINA project (see module 0), the injection of CO<sub>2</sub> into a

**Fig. 14** Chloride concentration distribution in quaternary aquifer (mg/l) after  $t = 50a$



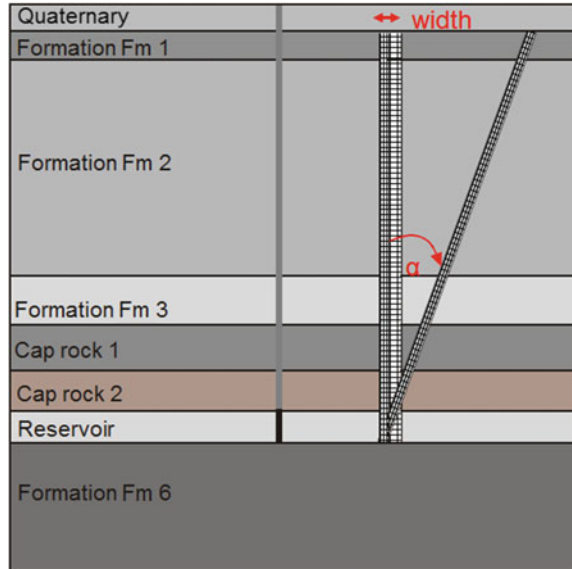
**Fig. 15** Fluid density distribution in quaternary aquifer ( $kg/m^3$ ) after  $t = 50a$



saline aquifer was simulated for 25 scenarios (see module A). For this purpose, the intrinsic permeability of the reservoir was varied between  $10^{-14}$  and  $10^{-12} m^2$  and that of the fault zone between  $5 \times 10^{-13}$  and  $10^{-10} m^2$ . The initial porosity was 25 %. The pore pressure increases, as determined by module A, were imported into the geo-mechanical model in form of a one-way hydro-mechanical coupling as a time function. A maximum pore pressure increase of approximately 0.25 MPa at the lower end of the fault zone was reached.

As a first approximation, a 2D plane strain geo-mechanical simulation was used. To prevent influences of the boundaries, the synthetic model was extended to a width of 30 km. For the simulations 4-node plane strain elements were used. Ideal elastic, ideal plastic material behavior and the Mohr-Coulomb failure criterion were assumed. The 40 m wide fault zone was modelled with solid finite thickness elements as

**Fig. 16** Synthetic model applied in the present study (personal communication Adams, 2014). The fault width ( $\Delta b$ ) and the inclination angle  $\alpha$  have been marked in red in the figure

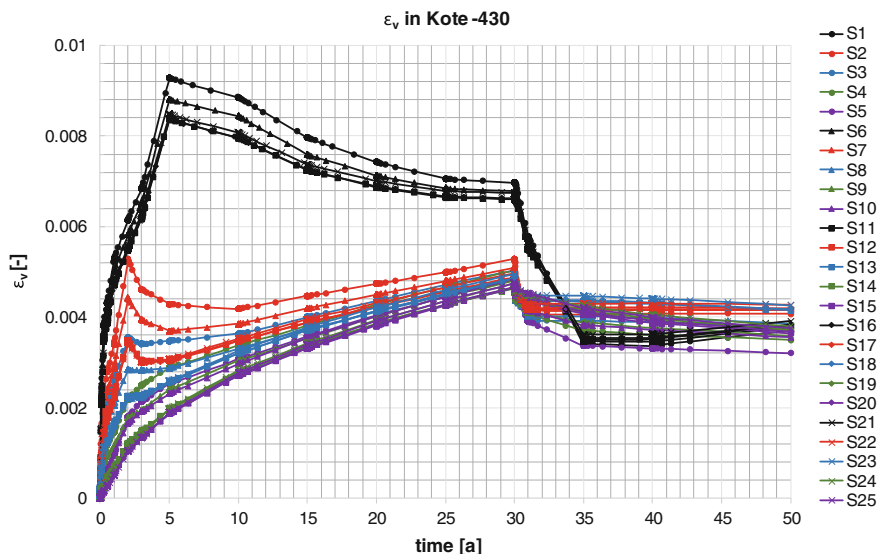


recommended by Cappa and Rutquist (2011), Gudmundsson et al. (2010) and Faulkner et al. (2010). Detailed information of the boundary conditions used the geometry and the rock parameters of the model are given by **personal communication Adams 2014**. A cross section of the synthetic model is shown in Fig. 16.

Exemplary, the changes of the opening width of the fault zone, also called hydraulic aperture  $\Delta b$ , as calculated for the 25 scenarios, are shown in Fig. 17. The results were generated at a calculation node in cap rock 2 as a function of time. Due to the high transmissivity of the fault zone, the maximum aperture was determined for scenario S1 to only about 3.5 mm. As the fault zone was modelled as porous media, this aperture equates to a very small volumetric strain of 0.009 which in fact doesn't result in a significant increase of the intrinsic permeability. Therefore, a fully hydro-mechanical coupling was not necessary. Furthermore, only elastic deformations of the fault zone and the reservoir occurred.

Volumetric strains as a function of time at certain depths of the fault zone were delivered to module 0 as input data for the risk assessment software.

Furthermore, a parametric study with hydro-mechanical single phase flow simulations was executed in the frame of module F to determine the conditions for which the volumetric strains of the fault zone are relevant regarding a fully hydro-mechanical coupling. Therefore, the transmissivity of the fault zone was reduced and the inclination was varied between 0° and 20°. The reduction of the transmissivity by 50 times leads to a maximum pore pressure increase of approximately 1 MPa at the foot of the fault zone, which is four times higher than in the 25 scenarios discussed above. In combination with an inclined fault zone, this pore pressure increase leads to a plastification of the fault zone, which causes volumetric



**Fig. 17** Hydraulic aperture  $\Delta b$  of the fault at 430 m depth (personal communication Adams 2014), The different parameter combinations of reservoir permeability and initial fault permeability represent the scenarios S1–S25

strains up to 0.037. This results in an increase of the intrinsic permeability in about one order of magnitude.

Taking the results of the parametric study into account (**personal communication Adams 2014**) it can be summarized that significant volumetric strains, which require fully coupled hydro-mechanical simulations, only occur when plastification in the fault takes place.

## 2.8 Module (H) Flexible Interfaces

Because the general goal of the CO<sub>2</sub>RINA-project was the development of a generalized methodology, the incorporated processes are not complete. To be able to incorporate additional processes, there should be the possibility to incorporate additional processes or models. This can be done in two ways: Internal coupling/refinement of process models or external coupling of models for additional risk pathways.

External coupling means, that the results of a simulation, i.e. concentrations or mass fluxes can be used as primary input for an additional model. One example is the CO<sub>2</sub> which leaks to the surface can be used as input for any kind of near surface atmospheric transport model.

Internal coupling means, that process parameters may change due to the incorporation of additional processes. This kind of coupling was demonstrated by

incorporation of the effect of microbiological processes onto the porosity and permeability of the reservoir rocks which has been extensively investigated in the project CO<sub>2</sub>BIOPERM (Hoth et al. this volume). The example is described there more extensively.

For the reservoir a simple form of the transfer function reads:

$$T\{\dot{m}_{inj}(t), K_{res}, K_{fault} \longrightarrow \text{transfer } \dot{m}_i(t), p_i(t), S_i(t)\}$$

with the abbreviations:

- $\dot{m}_{inj}(t)$  injection rate
- $K$  permeability
- $\theta$  porosity
- $\dot{m}_i$  mass flux through leakage i
- $p_i(t)$  pressure at point i
- $S_i(t)$  saturation at point i

On the other hand side, for the microbiological effects there can be derived a transfer function which changes the average porosities and permeabilities due to the effect of microbiological processes. This transfer function reads:

The transfer function for  $K$  and  $\theta$  to incorporate microbiological effects can be written:

$$T\{K, \theta, [c_\alpha(t)] \longrightarrow \text{transfer } \tilde{K}(t), \tilde{\theta}(t)\}$$

with the abbreviations:

- $[c_\alpha(t)]$  vector of concentrations
- $\tilde{K}(t)$  resulting average permeability
- $\tilde{\theta}(t)$  resulting average porosity

The combination of both functions results in a new transfer function, in which microbial processes are incorporated:

$$T\{\dot{m}_{inj}(t), \tilde{K}_{res}(t), \tilde{K}_{fault}(t) \longrightarrow \text{transfer } \dot{m}_i(t), p_i(t), S_i(t)\}$$

By using this approach, the results of the CO<sub>2</sub>BIOPERM project can be integrated into the CO<sub>2</sub>RINA methodology.

### 3 Results and Conclusions

The selection of appropriate kinds of independent variables and transfer functions (=interfaces between the modules) was a major challenge. This has to be done for each coupling specifically.

Example for the transport in an alluvial aquifer: Transfer from inflowing mass flux at point  $r_1$  to concentration at point  $r_2$  by using convolution integral (aquifer—module E):

$$c(t) = \int_{\tau=0}^{\tau=t} T \left\{ t - \tau, \dot{m}(\tau) \xrightarrow{\text{transfer}} c \right\} * \dot{m}(\tau) * d\tau$$

Transfer function for constant mass fluxes:

The concentration has to be calculated for a set of constant mass fluxes in the related module (aquifer model in this example) which are the base for interpolation.

$$T(X_1, X_2, \dots, X_N \xrightarrow{\text{transfer}} Y_1, Y_2, \dots, Y_N)$$

The approach is valid for several independent variables  $X_1, \dots$ , and dependent variables  $Y_1, \dots, Y_M$  by interpolation in a multi-dimensional space.

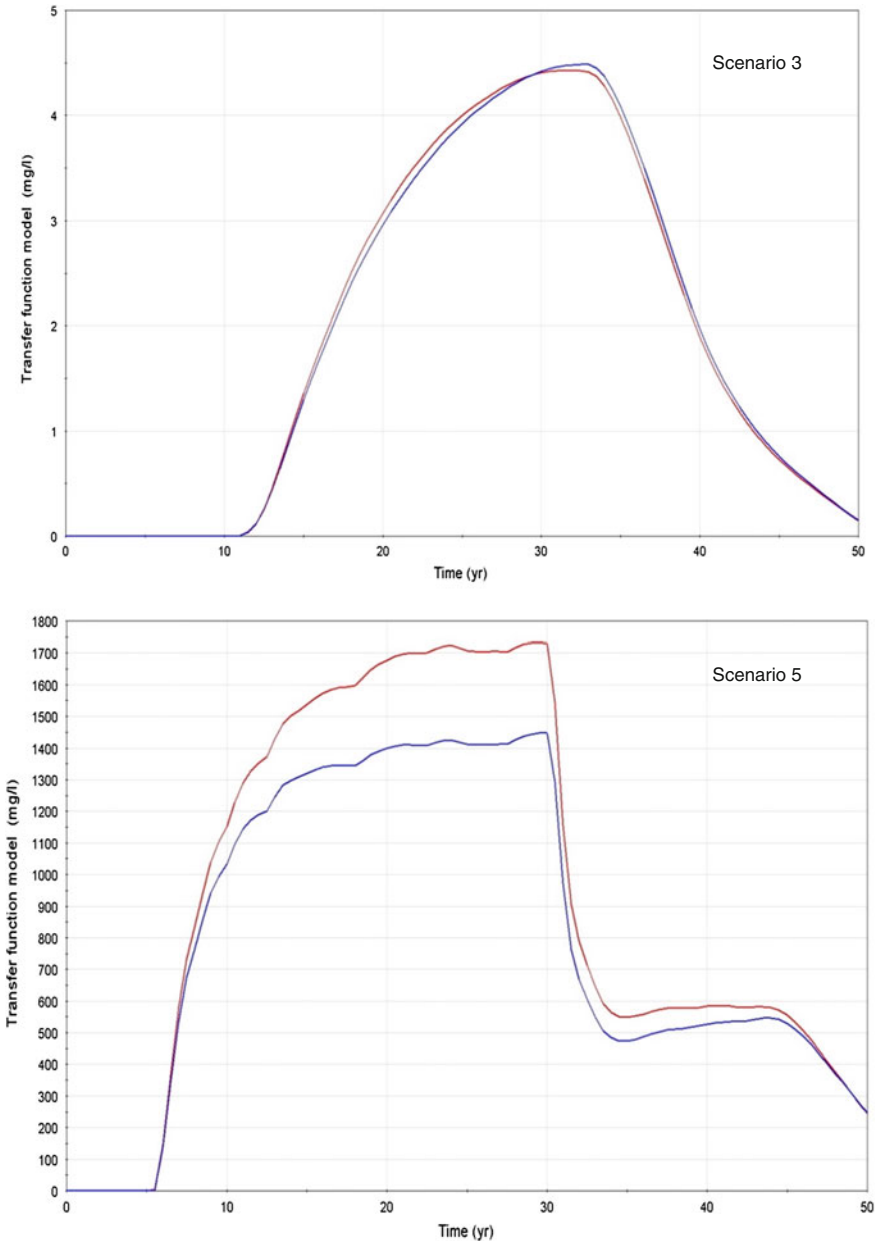
$$\dot{m}_i : T \left\{ \tau, \dot{m}_i(\tau) \xrightarrow{\text{transfer}} c \right\} = \frac{1}{\dot{m}_i} \frac{d}{d\tau} c(\tau, \dot{m}_i)$$

The validation of the approach by comparison of the overall model which was developed in module (A) with the coupling concept has been demonstrated at different examples. In Fig. 18 there is shown a benchmark calculation with the overall model for the reservoir, the fault and the alluvial aquifer in one model on the one hand side and the models coupled with transfer function on the other hand side for two different parameter scenarios. Figure 19 shows preliminary results regarding the incorporation of geomechanical effects.

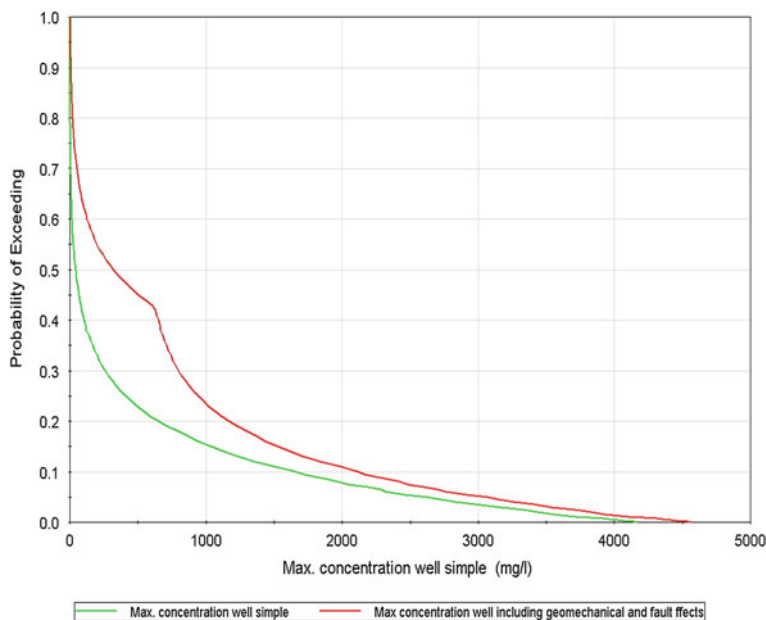
The following conclusions can be derived from the work:

- The methodology was implemented and extensively tested
- Most of the interfaces work properly
- Some instabilities for coupling reservoir model and fault model via pressure and saturation
- A new coupling concept was developed and has to be completely implemented and tested
- The iterative coupling of reservoir model and geomechanical model is difficult to be handled
- A new coupling concept for geomechanical effects has been developed and has to be implemented and tested as well
- Implications to coupling of other modules have to be evaluated

The developed methodology is very general and a universal base for risk assessment which has to be adapted to a specific site. It can be adapted to each level of investigation and continuously improved.



**Fig. 18** Leakage through fault and migration in shallow aquifer—comparison between direct implementation in the overall model (*red*) versus an implementation by transfer functions for two different parameter scenarios. *Upper part*—scenario 3 for a low fault permeability and *lower part*—scenario 5 for a high fault permeability. For low concentrations the coupling shows very consistent results, while in scenario 5 with high concentrations there are differences between the two approaches up to about 20 %



**Fig. 19** Probability distribution for CO<sub>2</sub>-concentration in a groundwater production well—comparison: *green* reservoir model + aquifer model, *red* reservoir model + fault model + geomechanical model + aquifer model. The difference between the distributions show the additional contributions of a detailed fault model and the incorporation of geomechanical effects

With required adaptations it can be applied to similar application fields in the use of the underground like:

- storage of hydrogen and natural gas
- deposition of brine and final waste deposits
- primary production of geothermal energy, especially petrothermal energy and production of shale gas

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