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The effect of providing details to the model of a geological structure on the assessment of CO_2 storage capacity

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Abstract: Massive emissions of CO_2 into the atmosphere are the most direct reason causing global warming and climate change, so more and more countries are starting to focus on carbon abatement technologies. In recent years, the method GCS (Geological Carbon Storage), injecting the CO_2 in a supercritical state underground for storage, is considered the most effective way to reduce greenhouse gas emissions. Saline aquifers are given special attention because of its huge amount of storage and, therefore, a deep saline aquifer is the best choice for the storage of CO_2. Exemplified by the well-explored Konary structure in the Polish Lowlands, results of assessments of CO_2 storage capacity are compared for three cases: (1) a simplified formula based on averaged geological and reservoir parameters and (2) a model of the structure based on averaged geological and reservoir parameters (homogeneous model) and (3) a model of the structure with more detailed geological data (including those on clay interbeds in the sandstone series of the reservoir horizon – heterogeneous model). This allows the estimation of how providing of details of geological and reservoir data, introduced into the model, can affect the ability of CO_2 migration within a reservoir horizon intended for CO_2 storage, and, consequently, also obtain a more accurate assessment of the capacity that the structure is capable of attaining.

Keywords: CO_2 storage coefficient, CO_2 storage efficiency factor, CO_2 capacity, CCS

INTRODUCTION

The concept of climate change mitigation by the use of underground carbon dioxide storage technology (GCS: Geological Carbon Storage) has been much discussed in recent years. Identification of geological structures (in this case especially saline aquifer structures) and the development of a methodology for estimating the CO_2 storage capacity of the structures are important factors in determining the efficiency of GCS. Most authors agree that the most accurate estimates of storage capacity are based on computer simulations of CO_2 injection into the geological structure. Due to the limited availability of data, averaged geological and reservoir parameters (thickness, porosity, permeability of the reservoir, and others) of the saline aquifer structure to which CO_2 is to be injected are usually adopted to estimate the capacity.

Numerous researchers (e.g.: Doughty & Pruess 2004, Pruess 2005, Ghanbari et al. 2006, Song et al. 2014, Ruprecht 2014, Zhang & Agarwal 2014) emphasize that for such modeling it is very important to take into account geological heterogeneity. For instance, Song et al. (2014) believe that a greater number of layers in the model will result in a better approximation of the actual situation in the saline aquifer, and will increase computation load. Permeability has an effect on the interface movement during the two-phase fluid displacement. The

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difference in the two-phase displacement interface positions will affect storage capacity (Song et al. 2014). Ghanbari et al. (2006) also believe that the presence of interbedding shales in a structure will have a large effect. CO_2 tends to become trapped beneath shale layers increasing thus lateral migration and decreasing vertical migration.

Based on the example of the well-explored Konary saline aquifer structure in Polish Lowlands, the paper provides a comparison of the results of assessments of CO_2 storage capacity for three cases: (1) calculations using a simplified formula based on averaged geological and reservoir parameters, (2) a model of the structure based on averaged geological and reservoir parameters (homogeneous model) and (3) a model of the structure with more detailed geological data (including those on clay interbeds in the sandstone series of the reservoir horizon – heterogeneous model). This comparison allows us to estimate how details of geological and reservoir data, introduced into the model can affect the evaluation of CO_2 migration within a reservoir horizon intended for CO_2 storage and, consequently, refine the assessment of the potential capacity of the structure.

GEOLOGY OF THE KONARY STRUCTURE AND CHARACTERISTICS OF POTENTIAL RESERVOIR HORIZONS

The Konary geological structure is located in central Poland between Inowrocław and Brześć Kujawski. The Konary anticline (a salt pillow) occurs on the north-western margin of the Kujavian Swell, within the Gniewkowo tectonic-structural unit, close to the boundary with the Mogilno-Uniejów Trough (Znosko 1969, Marek & Znosko 1972a, 1972b, Dadlez & Marek 1974). Konary and Ciechocinek salt pillows are present in the Gniewkowo region where the floor of the Zechstein strata lies at a depth of 5000–6000 m. Within these structures, salt has not pierced through the Mesozoic overburden (Feldman-Olszewska red. 2007, 2008).

Geological structure

The Konary anticline (Fig. 1) is situated between the Góra salt dome in the north and the Izbica Kujawska salt stock in the south (Dadlez et al. red. 2000). At the sub-Cenozoic surface, the anticline is marked by Tithonian, Berriasian and Lower Valanginian subcrops surrounded by upper Lower Cretaceous deposits and, in the southwestern limb, also by Upper Cretaceous rocks.

This anticline has been explored by a semi-detailed reflection seismic survey (about ten seismic profiles are located within the structure) and by a number of boreholes, including the deepest ones Konary IG-1 (total depth 3452.0 m to the Zechstein) drilled in the north-eastern limb (Marek red. 1974) and Byczyna 1 (total depth 5728.0 m to the Lower Carboniferous) drilled in the southeastern limb of the anticline.

The Konary anticline acquired its present-day form during regional inversion of the Kujavian Trough at the end of the Cretaceous and in the early Paleocene. Post-inversion erosion of the Gniewkowo Depression region removed Upper Cretaceous and upper Lower Cretaceous deposits to a depth of about 2500 m (Marek & Pajchlowa red. 1997, Dadlez 2001, Dziewińska et al. 2001, Krzywiec 2006). The degree of faulting of the Zechstein-Mesozoic complex is higher in its lower parts, decreasing upwards. The faults clearly fade out in the Lower and Middle Jurassic. They are also characterized by small amplitudes of fault slip.

By assuming conventionally that the elliptic-oval outline of the anticline is defined by the −800 m contour line of the top of the Lower Jurassic (Upper Toarcian), the length of the anticline is approximately 13 km, its width is about 6 km, and its area is around 80 km^2. A similar size of the structure is defined by the −1000 m contour line of the top of the Upper Pliensbachian: length 13–14 km, width 8 km, area about 112 km^2 (Tarkowski red. 2010, Tarkowski et al. 2011).

Reservoir horizons

The lithostratigraphic and hydrogeological analysis of the Mesozoic deposits of the Konary anticline shows that Lower Jurassic reservoir horizons are the most suitable for CO_2 storage (Tarkowski red. 2010, Tarkowski et al. 2011):

- reservoir horizon of the Borucice Formation of the Upper Toarcian,
- reservoir horizon of the Komorowo Formation of the Upper Pliensbachian.

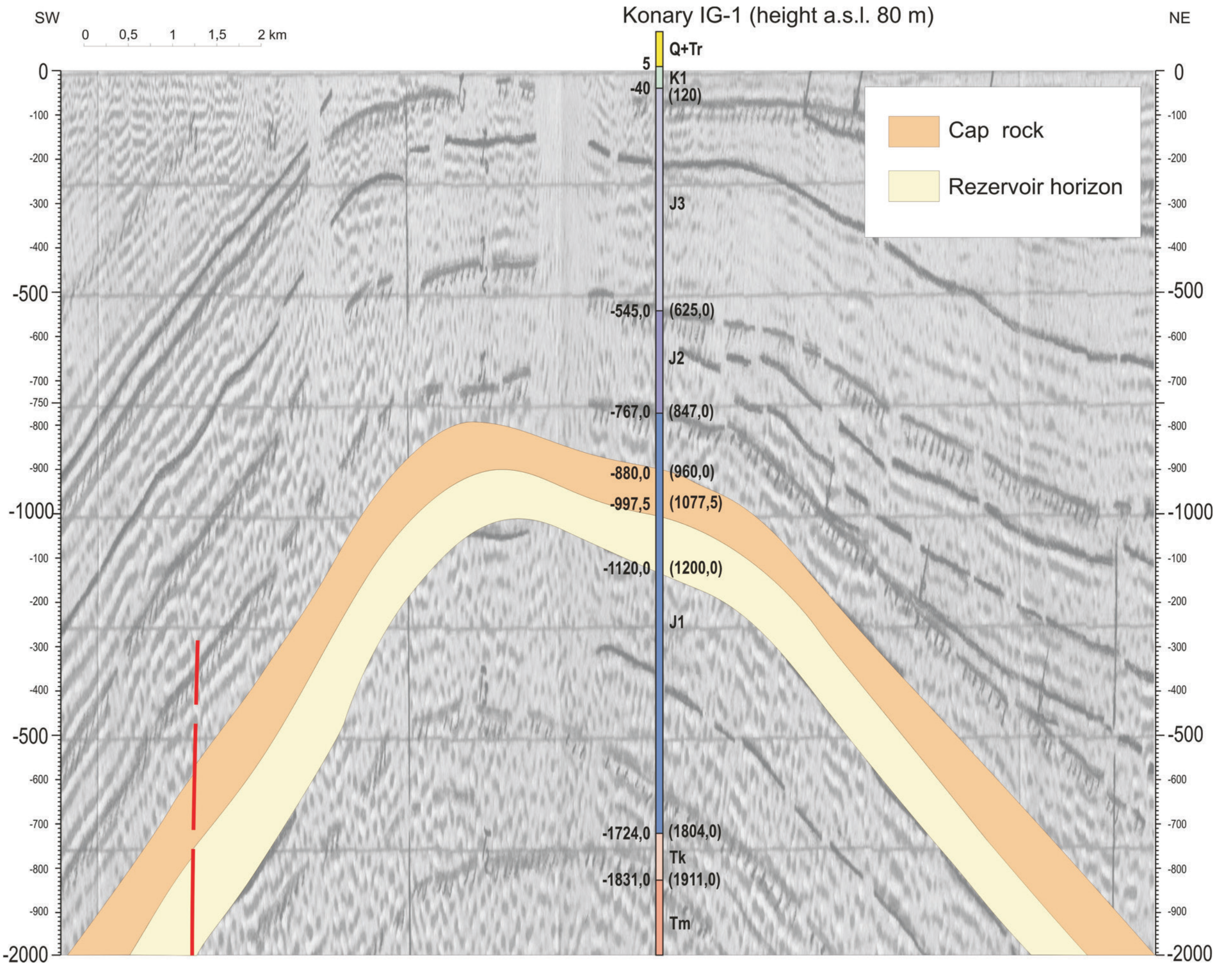

Fig. 1. *Cross-section through the Konary structure along Ciechocińska1-II/III-88/90 seismic line through Konary IG-1 well indicating the reservoir level: Komorowska formation, Upper Pliensbachian (Domerian) (Tarkowski et al. 2011)*

Both these formations provide favorable and very similar reservoir properties.

Reservoir horizon of the Borucice Formation was drilled through in the Konary IG-1 borehole at a depth of 847.0–960.0 m (113.0 m thick), and in the Byczyna 1 borehole at a depth of 1497.0–1702.5 m (205.5 m thick). It is represented by fine-grained sands, locally medium-grained, with claystone-mudstone interbeds which are more numerous in the upper part of the section. The thickness of the Borucice Formation is highly variable, averaging 150 m. The Borucice Formation is sealed by Aalenian-Bajocian-Lower Bathonian deposits represented by alternating series of claystones, mudstones, and subordinate sandstones, with a total thickness of approximately 200 m.

The reservoir horizon of the Komorowo Formation was drilled through in the Konary IG-1 borehole at a depth of 1077.5–1200.0 m (122.5 m thick), and in the Byczyna 1 borehole at a depth of 1812.0–1917.0 m (110.5 m thick). In its lower part, the Komorowo Formation is represented by fine-, medium- and coarse-grained sandstones, while its upper part includes a greater amount of clay-based rocks.

Deposits of these formations yield chloride-calcium brines of class I with mineralization of 42–49 g/dm^3 (cf. Bojarski red. 1996, Górecki et al. 2010).

The sandstone-dominated Komorowo Formation is sealed by the Ciechocinek Formation of the Upper Toarcian with an average thickness of 125 m. The Ciechocinek Formation is dominated by claystones and mudstones with interbeds of fine-grained sandstones, occasionally with calcareous-dolomitic or siderite cement.

CAPACITY ASSESSMENT FOR AVERAGED VALUES OF FORMATION PARAMETERS

Methods used in the calculation of the CO_2 storage capacity are different, but they are all based on the estimate of the pore volume in the reservoir horizon considered for the storage of carbon dioxide. This volume estimate involves a coefficient determining the portion of the pore volume that can be used to store CO_2. It is called storage efficiency. In this paper, the theoretical mass of carbon dioxide (G_{CO_2}) possible for CO_2 storage was calculated from the formula (1) (Gorecki et al. 2009, Goodman et al. 2011, U.S. Department... 2012, Sopher et al. 2014):

$$G_{CO_2} = A \cdot h \cdot \phi \cdot \rho_{CO_2} \cdot E \tag{1}$$

This is the most frequently used volumetric approach that allows the calculation of the mass of stored carbon dioxide (G_{CO_2}), based on: area (A), average thickness (h), average porosity (ϕ), and average density of carbon dioxide (ρ_{CO_2}) taking into account the storage efficiency coefficient (E). Its value (determined for a given geologic structure) differs depending on the author, ranging from 1 to 60%. In the calculations presented in this paper the value for the anticline under study is assumed to be 10%, and the thickness of the sandstone bed was reduced by 20% to account for the presence of clayey interbeds, obtaining the average CO_2 storage capacity for the Komorowo beds within the analysed geological structure to be 75.9 million tonnes (Tab. 1) (Tarkowski et al. 2011).

Table 1
Reservoir data on the Konary anticline (Komorowo Formation) (Tarkowski et al. 2011)

Parameter	Value
Size of area (A)	112 km^2
Average thickness (h)	110 m (80% = 88.0 m)
Average porosity (ϕ)	10%
Average pressure (P)	157.3 bar
Average temperature (T)	316.9 K
Average density of carbon dioxide (ρ_{CO_2})	770 kg/m^3
Storage efficiency coefficient (E)	10 %
Capacity	75.9 Mt

MODELLING

Methodological assumptions

Numerical modelling was performed using PetraSim (Thunderhead Engineering 2012) software with a TOUGH2 (Pruess et al. 1999) simulator with an ECO2N (Pruess 2005) fluid property module that was designed for applications to geologic sequestration of CO_2 in saline aquifers. This includes a comprehensive description of the thermodynamics and thermophysical properties of H_2O-NaCl-CO_2 mixtures. Flow processes can be modeled isothermally or non-isothermally, and phase conditions represented may include a single (aqueous or CO_2-rich) phase, as well as two-phase mixtures. Fluid phases may appear or disappear in the course of a simulation, and solid salt may precipitate or dissolve. The ranges of parameters for the model operation are as follows: temperature up to 100°C, pressure up to 600 bar, and salinity from zero to full saturation. These parameters should be adequate to most conditions encountered during CO_2 storage in deeply seated aquifers (Pruess 2005).

It is assumed that carbon dioxide is injected in a supercritical state, so that it has a much lower density and viscosity than the liquid brine it displaces. In situ, the supercritical CO_2 partitions between an immiscible gas-like phase and a phase of aqueous solution, according to an extended version of Henry's Law, yielding a multi-phase, multicomponent system. As in the vadose zone, strong gravity-driven flow occurs that is very sensitive to geologic heterogeneity and leads to the potential for nominally vertical flow (liquid infiltration in the vadose zone, the buoyant flow of CO_2 here) that is controlled by preferential flow paths. Also, as in the vadose zone, the mobilities of the flowing phases depend strongly on multi-phase flow effects at the pore scale, as embodied in continuumscale (i.e., model-scale) relative permeability functions that are often poorly known for a particular field site or fluid composition. Chemical reactions between CO_2 and rock minerals, as well as the dissolution of carbon dioxide in the brine that could potentially contribute to mineral trapping of CO_2, are not considered. Due to a lack of data on two-phase flow properties of supercritical CO_2 and liquid brines, generic characteristic curves are used: van Genuchten for liquid relative permeability and capillary pressure and Corey for gas relative permeability (Doughty & Pruess 2004).

Numerical model of the Konary structure

The development of the numerical model of the Konary structure was based on a static model comprising Lower Jurassic deposits (reservoir horizon of the Komorowo Formation) and their cap rocks. The shallower reservoir horizon of the Borucice Formation is not involved here. The boundary of the model is accepted in such a way as to cover the whole structure. The model is block-shaped, about 14 km × 8 km × 1.5 km in size. Based on structural maps (Tarkowski et al. 2011), contours have been digitized using Surfer software, to which specific values have been assigned. On the basis of the data sheet XYZ, a regular grid of values (so-called gridding) has been developed. The kriging method was used for interpolation, which allows determining the values at regular grid nodes based on irregularly spaced points of the independent variables XY and on the values of the function Z.

To determine the geological properties (thickness, porosity, permeability and density of deposits) of the Komorowo Formation intended for CO_2 storage, and of the impermeable cap rocks, data from interpretation of well logs in the Byczyna-1 borehole have been used for the construction of the detailed model (based on: *Kompleksowa interpretacja*... 1989).

Taking into account the need for an appropriate number of blocks in the model grid to carry out the most accurate calculations and simulations of CO_2 injection in the deposit, and the constraint resulting from the software used, a polygonal grid was employed for the construction of the model. It uses the Voronoi method of cell division. The model boundaries in TOUGH2 are closed. However, by giving very large volumes (about 1×10^{50} m^3) to the boundary cells of the grid, these boundaries could be apparently "open" (Pruess et al. 1999). The vertical grid of the model reflects the lithology of strata. After the grid refinement for the CO_2 injection modelling, the Komorowo Formation has been divided into 12 layers. In the first case (homogeneous model) these layers have the same averaged parameters: permeability 500 mD, porosity 10% and rock density 2.43 g/cm^3. In the second case (heterogeneous model) these 12 layers differ in their characteristics as regards the reservoir parameters (Fig. 2, Tab. 2). Each of these facies corresponds to a material type in TOUGH2, and as such has its own set of flow properties. Overall, permeability of the storage formation varies by nearly two orders of magnitude among material types, making the preferential flow a significant effect, especially when coupled with the strong buoyancy forces acting on the gas-like CO_2 plume.

For the impermeable cap rocks, a single geological layer has been assumed, which has averaged geological and hydrodynamic properties and is divided into five equal parts (five cell layers) with the same parameters: permeability 0.08 mD, porosity 10% and rock density 2.43 g/cm^3.

The horizontal grid shows the outline of the structure. It has been extended by approximately 1 km outward to make the apparently open boundary removed from the outer contour of the reservoir (with potential spill points) and to observe if CO_2 does not reach a spill point. The yellow line shows this outer limit that CO_2 should not cross. The grid was made denser near the outer contour of the reservoir and close to the injection boreholes (Fig. 3).

Modelling assumptions

It has been assumed that the injection occurs through the entire thickness of the Komorowo Formation by four vertical boreholes whose locations were determined by a trial-and-error procedure to maximize the amount of CO_2 that could be injected. Flow into each cell that the well intersects is apportioned by $k \cdot h$ (permeability × height). The total $k \cdot h$ is calculated for the entire well and then the flow into each cell is determined by the permeability and height (intersection length) for that cell. Injection simulation was carried out for a period of 30 years to fill in the structure completely. An additional simulation was performed for a period of 1000 years (after injection) to monitor the CO_2 plume migration to exclude the possible migration of the injected carbon dioxide outside the structure. The initial conditions, inputted into the model, are as follows: pressure gradient 1.04×10^3 hPa/10 m; temperature gradient 2.9°C/100 m. In addition, brine mineralization is assumed to be 42 g/dm^3.

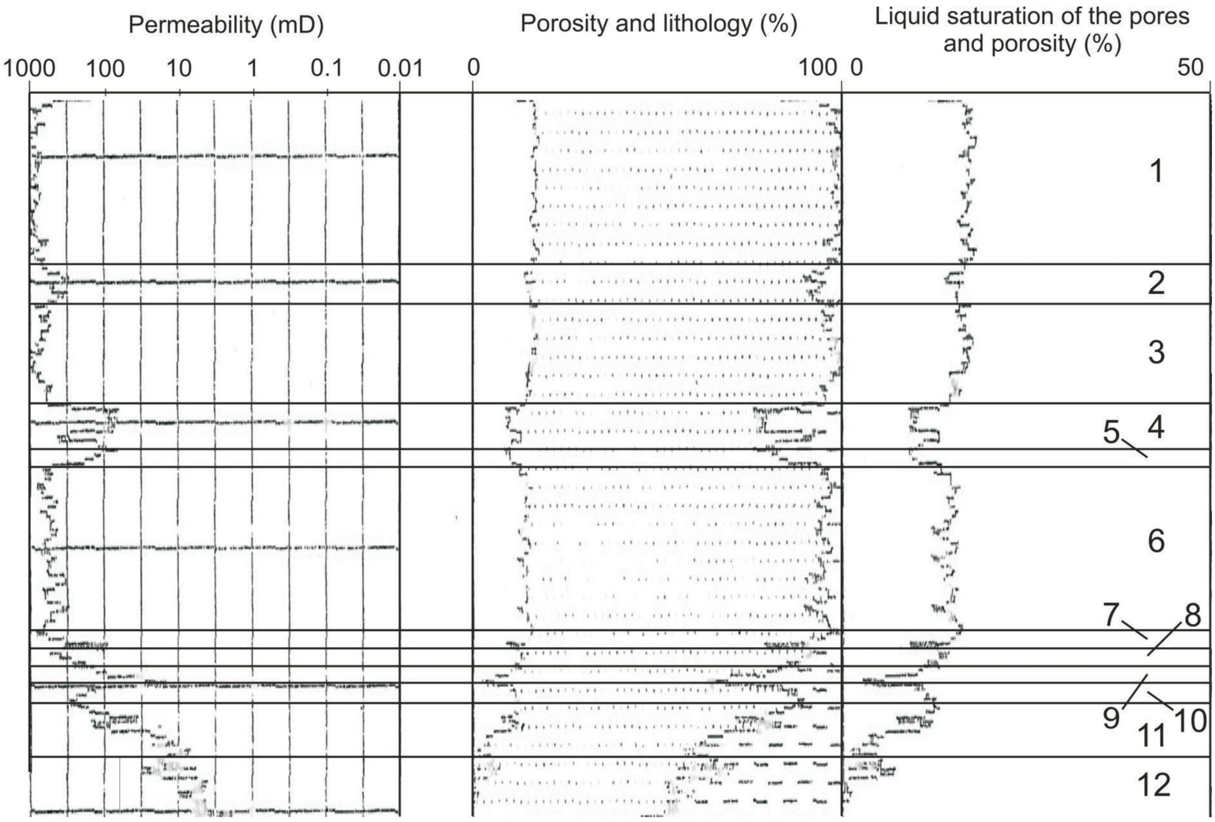

Fig. 2. *Well log used for determining layer properties from the Byczyna-1 well in depth interval 1832–1942 m (based on: Kompleksowa interpretacja... 1989)*

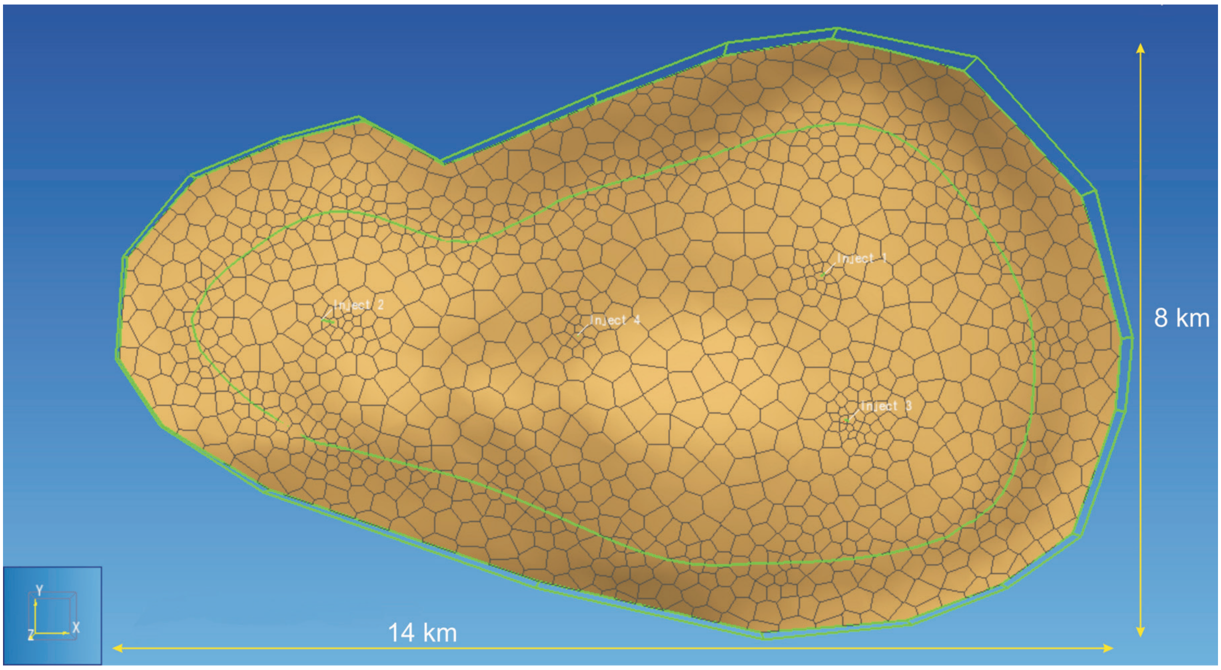

Fig. 3. *Konary Structure shape with marked injection wells (Inject 1, 2, 3, 4) and outer contour of the reservoir (with potential spill points)*

Table 2
Interbeds and their reservoir properties within the Komorowo Formation (Lower Jurassic) in the Byczyna-1 borehole (based on: Kompleksowa interpretacja... 1989)

No.	Thickness [m]	Contribution [%]	Permeability [mD]	Porosity [%]	Rock density [g/cm^3]
1	28	25	900	17	2.5
2	5	5	300	16	2.49
3	16	14	700	17	2.51
4	7	6	60	10	2.57
5	3	3	100	10	2.57
6	24	22	400	14	2.5
7	2	2	90	10	2.57
8	2	2	300	10	2.57
9	3	3	10	3	2.57
10	4	4	200	10	2.57
11	9	8	20	7	2.49
12	7	6	10	3	2.49

RESULTS

From the viewpoint of storage efficiency or keeping the pressure increase low enough to ensure safe storage, optimum conditions for filling the structure with carbon dioxide were achieved in four vertical boreholes with the flow rates determined by a trial-and-error procedure.

In the first case (homogeneous model) flow rates are: 37 kg/s in the Inject 1 borehole, 15 kg/s – Inject 2, 24 kg/s – Inject 3, and 25 kg/s – Inject 4. In total, it gives 101 kg/s, 3.18 million tons per year and about 95.6 million tons CO_2 during the 30-year injection period. In the second case (heterogeneous model) the flow rates are the following: 50 kg/s in the Inject 1 borehole; 30 kg/s – Inject 2, 37 kg/s – Inject 3, and 31 kg/s – Inject 4. Overall, it gives 148 kg/s, which is over 4.7 million tons per year. For the 30-year period, it is 140 million tons of injected carbon dioxide. After the injection of $CO_{2,}$ the gas first spreads around the boreholes. Then, the characteristic anticlinal shape of the geological structure (in this case it is a "saddle"), and the fact that supercritical CO_2 is less dense than the saline formation waters into which it is injected, cause the CO_2 to rise through the formation. In the second case (heterogeneous model) its rate of ascent, however, is limited by the presence of shales with relatively low permeability (Fig. 4).

To examine the long-term processes that occur within the structure under study, and to find out if the CO_2 will not leak out (laterally and vertically) beyond the structure after the injection is completed, additional simulation of "monitoring" was carried out for all discussed variants over the next 1000-year period after completion of the injection. As a result of the simulation, continuous upward migration of free CO_2 was observed along the near-top layers to the local summit of the structure. At the amount of the injected gas, no CO_2 leak has been observed.

DISCUSSION

Because of the presence of the shale layers, CO_2 tends to become trapped beneath them, thus increasing the lateral migration. This results in the formation of horizontal preferential flow paths of carbon dioxide. Because of the occurrence of such preferential flow paths, CO_2 migration along them is intensified and consequently carbon dioxide can reach faster the delimited boundary of the structure (spill point), beyond which it can leak out. On the other hand, the occurrence of interbeds with various flow properties (clay interbeds in a series of sandstones) can lead to a more complete fill of the structure with CO_2 that rises up by the forces of buoyancy. This is because the CO_2 is accumulated not only at the top of the whole structure, from where it migrates laterally reaching its boundary, but also beneath every interbed of low-permeability rocks, and it moves on either side along the numerous interbeds (Figs 4, 5). Accordingly, the estimated carbon dioxide capacities for the same structure, calculated by averaging the reservoir parameters or taking into account clay interbeds in sandstones, may vary.

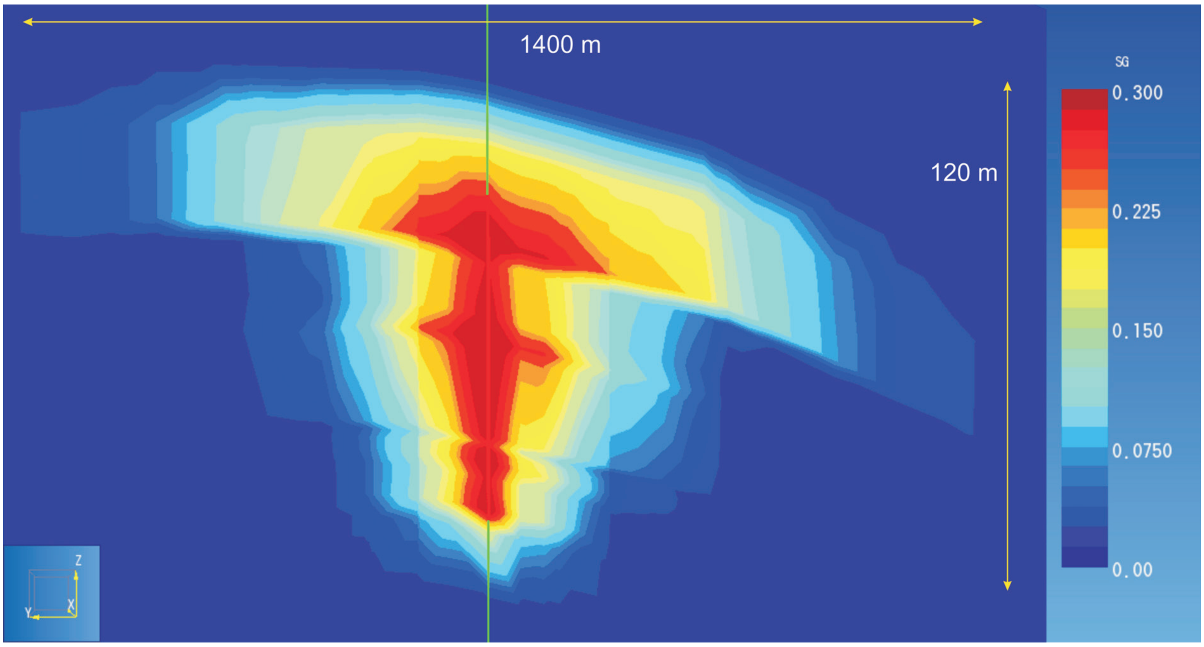

Fig. 4. *Cross-section of gas saturations after 8 months of CO_2 injection (shows forming preferential flow paths between the shale layers)*

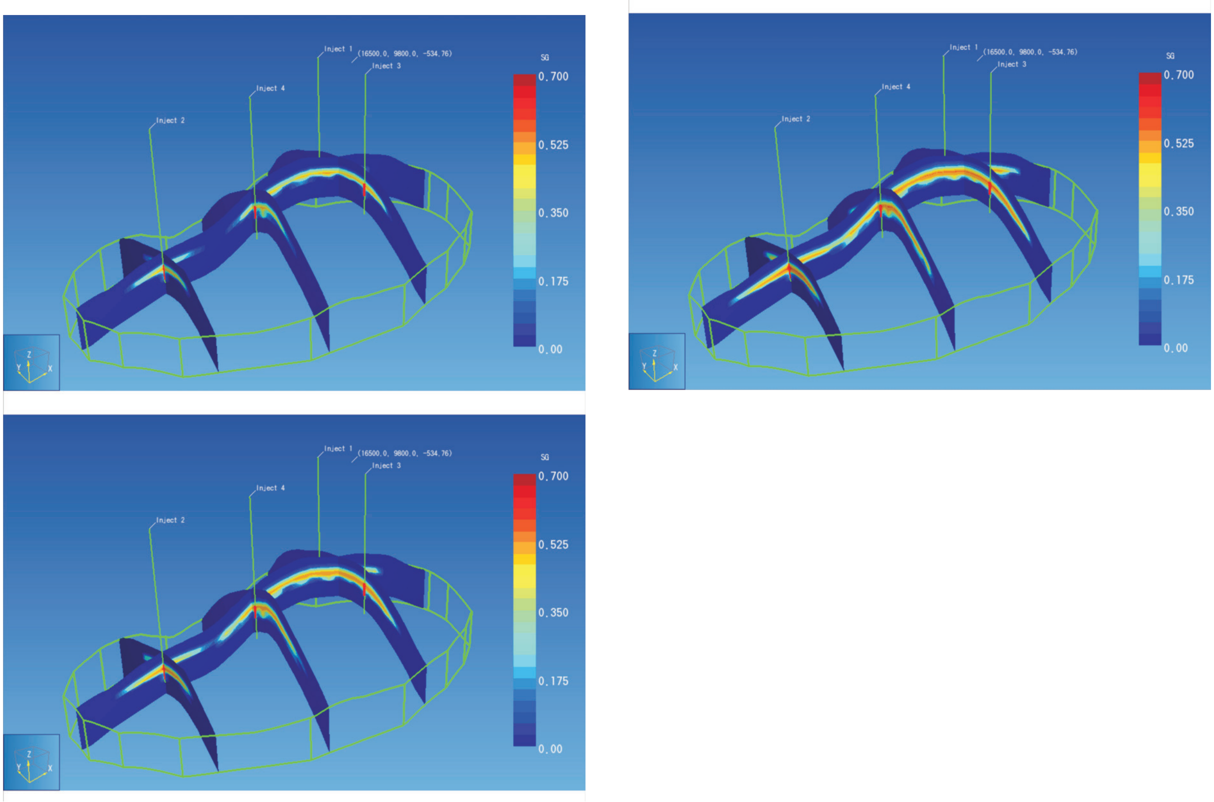

Fig. 5. *Distribution of CO_2 saturation in detailed (heterogeneous) structure after 10, 20, and 30 years of injection (XYZ model dimensions: about 14 km × 8 km × 1.5 km)*

Such a difference was found when calculating the storage capacity of the Konary structure. The capacity calculated using the formula given by equation (1) that involves averaged reservoir parameters (also named static or volumetric capacity) amounted to 75.9 million tons, while the storage capacity calculated by the modeling that involves clay interbeds amounted to 140 million tons (Tab. 3).

Table 3
Calculated CO_2 storage capacity and CO_2 storage coefficient for three cases

Cases	**Capacity [mln tonnes]**	**CO_2 storage coefficient [%]**
Formula (1)	75.9	10
Modelling (homogeneous model)	95.6	12.6
Modelling (heterogeneous model)	140	18

CONCLUSIONS

In this paper, a CO_2 storage scenario in a deep saline aquifer is presented, with an emphasis on the hydrodynamic trapping mechanisms. Rocks are naturally heterogeneous, and this has to be taken into account when modeling CO_2 storage. Different types of heterogeneities arise in different depositional environments.

In this study, we focus on the presence of interbeds that cause inflow properties (shale layers in a series of sandstones) to differ. In general, the shale layers prevent the vertical movement of the gas, and also prevent vertical downward movement of the water saturated with CO_2, so there is more lateral movement. The characteristic T-shape which develops in the homogeneous model is no longer present, and the CO_2-saturated brine seems to have a more uniform distribution in the regions invaded by the CO_2 gas. The presence of shales did, however, have a large effect. As the percentage of shale increases, the CO_2 gas tends to become trapped beneath the lower layers of shale and moves laterally rather than vertically.

The capacity of CO_2 storage for the structure of averaged geological and reservoir parameters was 75.9 million tonnes using the simplified formula, while that obtained as a result of carbon dioxide injection simulation to the model of the structure with detailed geological structure (involving clay interbeds in a series of sandstones) was 140 million tonnes (about twice as much). It means that the storage efficiency coefficient for the Konary structure assumed for calculations for the formula (1) is too low (underestimated) and should be 18%.

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