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Numerical simulation of hydrogen storage in the Konary deep saline aquifer trap

Glossary

UHS	–	underground hydrogen storage,
RES	–	renewable energy sources,
P_{frac}	–	minimum fracturing pressure (Pa),
$\sigma_{H,min}$	–	minimum horizontal stress (Pa),
$\sigma_{H,max}$	–	maximum horizontal stress (Pa),
σ_{Tw}	–	tensile strength (Pa),
P_i	–	initial pressure in the structure intended for hydrogen injection, pore (reservoir) pressure (Pa),
η	–	poroelastic constant,
α	–	Biot coefficient (–),

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ν	– Poisson's ratio (–),
σ_V	– vertical stress,
ρ	– bulk density of overburden rocks (kg/m^3),
g	– the gravitational constant (m/s^2),
H	– depth (m),
$P_{\text{capillary}}$	– capillary pressure (Pa),
γ	– surface tension between hydrogen and brine (N/m),
θ	– contact angle of the hydrogen-brine-rock system ($^\circ$),
R	– characteristic pore space radius of the caprock (m),
Mg	– Mega gram – $1,000,000 \text{ g} = 1,000 \text{ kg}$,
Total capacity	– the total amount of hydrogen injected into the structure during the 2, 3 or 4 years of the initial filling period with various flow rates not exceeding allowable pressures and the spill point,
Working gas	– the amount of hydrogen that can be withdrawn within six-months from the storage at a given hydrogen flow rate (time-weighted flow rate average from the initial injection period),
Cushion gas	– the capacity difference between total capacity and working gas.

Introduction

At present, hydrogen is being considered as an energy carrier for fossil fuel-based energy (Fonseca et al. 2019; Abdin et al. 2020; Noussan et al. 2021). A hydrogen economy is an important tool for achieving climate neutrality (Hanley et al. 2018; Tagliapietra et al. 2019). It is assumed that in several years, hydrogen will be an essential energy carrier in the chemical, metallurgical, and transport industries, and in the long term, in the aviation and maritime sectors (The Future of Hydrogen 2019; Arenillas et al. 2021) and EU Parliament Communication (COM/2020/301 2020).

Nowadays, hydrogen is produced from fossil fuels but can be made using renewable energy sources through the electrolysis of water (green hydrogen) (Noussan et al. 2021; Olabi et al. 2021). However, most renewable energy sources, such as wind and solar sources, are characterized by intermittent energy production, and in addition, the demand and production for energy do not necessarily coincide. Thus, there is a need to store surplus energy during periods of increased supply, in order to supplement shortages during periods of increased demand. Energy generation from RES in the form of hydrogen produced through the electrolysis of water will ensure the sustainability of energy supply and demand in the near future and increase energy security (Matos et al. 2019; Noussan et al. 2021; Schultz et al. 2023). One of the significant problems in developing the hydrogen economy, as pointed out by Amirthan and Perera (Amirthan and Perera 2022), is the development of appropriate systems for its storage, whether on the surface of the earth or in appropriate deep, underground geological structures (traps).

Hydrogen has a low energy density by volume; therefore, significant capacity is needed for its large-scale storage. Such possibilities are identified with regard to appropriate geological structures (deep saline aquifers, depleted hydrocarbon fields, salt caverns) resulting in underground hydrogen storage (UHS) being considered today (Tarkowski 2017, 2019; Zivar et al. 2021; Aftab et al. 2022). Several recent studies in this area have presented the perspectives and barriers facing the implementation of UHS technology on an industrial scale: Tarkowski and Uliasz-Misiak (Tarkowski and Uliasz-Misiak 2022), Hematpur et al. (Hematpur et al. 2023), Raza et al. (Raza et al. 2022), Thiyagarajan et al. (Thiyagarajan et al. 2022) and Jafari Raad et al. (Jafari Raad et al. 2022).

1. State of the Art in hydrogen storage

The effects of caprock capillary pressure and fracturing pressure are often raised in the context of UHS (Reitenbach et al. 2015; Iglaue 2022). For reasons of safety, Sainz-Garcia et al. (Sainz-Garcia et al. 2017) suggest adopting a minimum value of caprock capillary pressure in hydrogen storage facilities.

Okoroafor et al. (Okoroafor et al. 2022) analyzed the scenarios of injecting, storing and withdrawing hydrogen using storage simulations. The obtained results allowed them to propose criteria for selecting locations for UHS in depleted natural gas deposits. The results of Ershadnia et al. (Ershadnia et al. 2022) suggest that hydrogen recovery is successful if the aquifer is more anisotropic and has a lower temperature and low density and if viscosity cushion gas is injected prior to hydrogen storage.

UHS requires cushion gas, which enables the maintenance of sufficiently high pressure during the operation of underground storage. It also affects the efficiency of working gas injection and withdrawal. Heinemann et al. (Heinemann et al. 2021), analyzing the results of injection, storage and hydrogen withdrawal in the geological structure of deep saline aquifers, indicate that the volume of cushion gas directly determines the efficiency of the injection and withdrawal of working gas. Using hydrogen underground storage in a heterogeneous sandstone reservoir, Mahdi et al. (Mahdi et al. 2021) examined the effect of caprock availability and hydrogen injection rate on the hydrogen withdrawal factor and hydrogen leakage rate. Their results indicate that both caprock and injection rate have an important impact on hydrogen leakage, and the quantities of trapped and withdrawn hydrogen. Tightness of caprock is very important for UHS as it prevents gas from leakage from underground storage (Ghaedi et al. 2023; Zeng et al. 2023).

Several publications indicate the impact of the initial filling of the UHS operation on the efficiency of its gas injection and withdrawal process. Feldmann et al. (Feldmann et al. 2016) presented a numerical simulation of a depleted gas field, assuming that the storage was initially filled with hydrogen for five years, and seasonal hydrogen injection and withdrawal were performed for the next five years. The results showed that the critical aspects are the hydrodynamic behavior of hydrogen and its interaction with residual fluids in storage. Other

articles (Pfeiffer et al. 2016, 2017) showed the results of the initial filling of underground storage with nitrogen as a cushion gas and hydrogen, and the impact on storage of breaks of several weeks followed by the injection and withdrawal of hydrogen. It was found that storage performance increases with the number of storage cycles and that the storage is mainly limited by the achievable extraction rates. In a subsequent paper, Pfeiffer and Bauer (Pfeiffer and Bauer 2019) assessed the usefulness of simulation models in determining the gas flow rate in the well and pressure changes. It was found that storage efficiency indicators (particularly the achievable storage flow rate) depend on the averaging schemes used when creating spatial models. Chai et al. (Chai et al. 2023) showed that multiple hydrogen injection/withdrawal cycles are useful for hydrogen storage, with an increase in efficiency in the last storage cycle and they also demonstrated that nitrogen as a cushion gas is more efficient than carbon dioxide.

It is emphasized that in the case of depleted natural gas fields, their significant advantage in terms of hydrogen storage relates to the presence of gas remaining in the field, which will act as cushion gas. The disadvantage is its negative impact on the purity of the withdrawn hydrogen (Amid et al. 2016; Zivar et al. 2021). Zivar et al. (Zivar et al. 2021) indicate that when planning to use a depleted gas field for UHS, it is essential to complete gas production at the right time, which will allow the construction of a storage facility at a lower cost and within a shorter time period, due to the existing infrastructure. The results of numerical simulations of seasonal hydrogen storage in hydrocarbon fields (Lysyy et al. 2021) show that the implementation of four annual hydrogen injection-withdrawal cycles, followed by one extended gas withdrawal period, facilitates a final hydrogen recovery rate of 87%.

A computer simulation of hydrogen injection, conducted for the Suliszewo structure (Luboń and Tarkowski 2020) and assuming that the fracturing pressure and caprock capillary pressure are not exceeded, showed that upconing causing large amounts of extracted water could be a significant obstacle to UHS. Luboń and Tarkowski (Luboń and Tarkowski 2021) analyzed the impact of caprock capillary pressure on the capacity of stored CO₂ and H₂. Analysis showed that the considered structure in terms of capacity is more suitable for the underground storage of H₂ than CO₂. Computer simulations of the UHS operation in a deep saline aquifer of the Suliszewo structure (Luboń and Tarkowski 2023) enabled the determination of influence of the time period of the initial filling with hydrogen and the impact of the depth on the subsequent operation of the UHS. The working capacity grew as the depth increased, reaching maximum values at depths of approximately 1,200–1,400 m.

1.2. Objectives

The research was intended to determine the conditions for the preparation and operation of UHS. This was performed by modeling the injection and withdrawal of hydrogen in the deep, Lower Jurassic saline aquifer of the Konary geological structure (trap). This

required: building a geological model of the structure under consideration; estimating the allowable pressures (fracturing and caprock capillary pressure); determining the time period of the initial hydrogen filling of the underground storage; modeling the thirty operation cycles of underground storage (gas injection and withdrawal). This type of research is essential when planning the use of the geological structure (trap) of the deep saline aquifer for UHS and allows us to determine the maximum flow rate of injected hydrogen, depending on the fracturing and caprock capillary pressure. Hydrogen flow rates are important for estimating total capacity, working gas capacity and cushion gas capacity. Modeling also allows us to determine the amount of water extracted during the cyclic withdrawal of hydrogen.

2. Materials and methods

The research was performed in accordance with the following scheme:

1. Building a geological model of the Konary structure.
2. Estimation of allowable pressures.
3. Simulation of initial hydrogen filling into the structure across three variants: 4, 3, and 2 years of initial filling.
4. Simulation of UHS operation (injection and withdrawal).

Building a geological model of the Konary structure. Simulations of hydrogen injection were performed in the PetraSim Transportation of Unsaturated Groundwater and Heat 2 (TOUGH2) software with the equation of the state 5 (EOS5) module (Pruess et al. 1999). The EOS5 module uses water, not brine, which can change rates of water production. This is a limitation of our research due to the capabilities of the available software. The implementation of the intended works required the construction of a geological model of a Lower Jurassic reservoir – the Komorowo formation of the Konary anticline. It is located in central Poland within the geological unit known as the Pomeranian-Kuyavian Swell. The indicated reservoir was previously considered for CO₂ storage (Tarkowski et al. 2011; Luboń 2020). Within the area of the Konary geological structure, drilling was carried out in two wells: in the Konary IG-1 well at a depth of 1077.5–1200 m (thickness 122.5 m) and in the Byczyna 1 well at a depth of 1832–1926 m (thickness 94 m). The reservoir consists of fine-, medium- and coarse-grained sandstones (~80%) with a larger share of clay rocks near the floor (Luboń 2020). Based on the Byczyna 1 well logs available in the Central Geological Database of the Polish Geological Institute (CGD PGI 2023), in the vertical section, the model of the reservoir was divided into ten layers, to which the determined values of porosity, permeability and density of rocks were assigned (Table 1). The divisions in the geological cross section were determined by fractional stratification, consisting in determining a constant proportion of individual strata in relation to the thickness of the entire stratigraphic sequence. Based on available data from the Byczyna-1 well, cross sections and a structural map of the Komorowo formation, isolines with specific depths were read. On the basis of the XYZ data

Table 1. Data used to create the Konary structure numerical model
 Tabela 1. Dane wykorzystane do utworzenia modelu numerycznego struktury Konary

No.	Depth (m)	Porosity (%)	Permeability (mD)	Rock density (kg/m ³)	Initial pressure (MPa)	Vertical stress σ_V (MPa)	Minimum and maximum horizontal stress $\sigma_{H,min} = \sigma_{H,max}$ (MPa)	Minimum value of fracturing pressure $\sigma_{f,min}$ (MPa)
1	682.68	16.75	900	2,500	7.4	16.74	9.03	13.86
2	699.18	16	330	2,490	7.57	17.08	9.23	14.09
3	709.68	16.63	725	2,510	7.68	17.47	9.41	14.24
4	721.18	9.86	63.57	2,570	7.8	18.18	9.7	14.40
5	726.18	10.33	101.67	2,570	7.85	18.31	9.77	14.47
6	739.68	14.08	435.42	2,500	8.0	18.14	9.78	14.66
7	752.68	9.5	90	2,570	8.13	18.98	10.12	14.84
8	754.68	10	300	2,570	8.15	19.03	10.15	14.87
9	757.18	3	10	2,570	8.18	19.09	10.18	14.90
10	760.68	9.5	195	2,570	8.21	19.18	10.22	14.95

sheet prepared in this way, a regular grid of values was determined (gridding). For interpolation, the kriging method is used. The mesh prepared in this way was imported into the PetraSim TOUGH2 software. In this software, a polygonal grid based on cell division by the Voronoi method was used to simulate hydrogen injection and withdrawal.

The other characteristics are: pressure gradient – 0.104 MPa/10 m (reservoir pressure 7.4–8.21 MPa), geothermal gradient – 2.9°C/100 m (reservoir temperature 35.8–48°C), brine salinity – 42 kg/m³, rock pores compressibility – 4.5^{–10} Pa, permeability in the vertical direction was 10% of the permeability in the horizontal direction (Tarkowski 2010; Luboń 2020, 2022). The reservoir is sealed from the top by layers of the Ciechocinek Formation of the Lower Toarcian, with a thickness of approx. 125 m. Clay-mudstone rocks may be found, with thin inserts of fine-grained sandstones. It was assumed that the overburden and the underlying layers were impermeable and not included in the model.

It was assumed that the injection and subsequent withdrawal of hydrogen would occur through one well located at the top of the Konary structure. The hydrogen would be injected and withdrawn throughout the entire thickness of the reservoir layer.

Estimation of allowable pressures: minimum fracturing pressure and caprock capillary pressure. The flow rates of the injected hydrogen were adjusted to the allowable pressures. The bottomhole pressure did not exceed the minimum fracturing pressure. The pressure in the top of the storage (i.e., in the roof section of the near-well zone and at the top of the structure) did not exceed the sum of the initial pressure and the caprock capillary pressure. It was assumed that, because the model in the roof is impermeable, and regardless of this pressure, the structure could become unsealed, which we would overlook during modeling. The injected hydrogen must not exceed the spill point of the structure. The fracturing pressure was estimated for the injection/withdrawal well located at the top of the Konary structure. If a significant increase in pore pressure due to hydrogen injection from the wellbore to the formation occurred, the equation below would be an estimate of the lower bound on P_{frac} (Carnegie et al. 2002):

$$P_{frac} = \frac{3\sigma_{H,min} - \sigma_{H,max} - 2\eta P_i + \sigma_{Tw}}{2(1 - \eta)} \quad (1)$$

$$\eta = \frac{\alpha(1 - 2\nu)}{2(1 - \nu)} \quad (2)$$

The values usually adopted for reservoir rocks of underground hydrocarbon storage are $\alpha = 0.7$ and $\nu = 0.25$ (Woźniak and Zawisza 2011). The same values were used in the presented research.

The minimum horizontal stress can be calculated according to the formula:

$$\sigma_{H,min} = \frac{\nu}{1 - \nu}(\sigma_V - \alpha P_i) + \alpha P_i \quad (3)$$

If we assume a constant value for the bulk density of the overburden rocks, the vertical stress is determined by the following equation:

$$\sigma_V = \rho g H \quad (4)$$

The calculations assumed that $\sigma_{H,\min} = \sigma_{H,\max}$. The tensile strength was accepted to be 6.45 MPa, the same as the average value obtained during the testing of reservoir rock samples of Polish natural gas in the “Swarzów” underground storage facility (Wóźniak and Zawisza 2011).

The caprock capillary pressure is also crucial, above which hydrogen, as a result of injection and buoyancy forces, may penetrate through the capillaries of the caprock. The capillary pressure is defined by the Young-Laplace equation (Cavanagh 2010; Tokunaga and Wan 2013):

$$P_{capillary} = \frac{2\gamma \cos(\theta)}{R} \quad (5)$$

The values for the cosine of the contact angle between hydrogen-brine-rock system and the surface tension between water and hydrogen were taken from Iglauer (Iglauer 2022). This presented the relationships from which these values can be calculated for the desired depth:

$$\gamma = 0.073 - 5.89286 \cdot 10^{-6} H \quad (6)$$

$$\cos\theta = 0.6784 - 0.0002 H \quad (7)$$

For safety reasons in relation to hydrogen storage, the minimum values of these pressures were taken into account.

Simulation of initial hydrogen filling into the structure across three variants: 4, 3 and 2 years of the initial filling. For the initial filling, three options were applied to the Konary structure: 4, 3, and 2 years of hydrogen injection. Luboń and Tarkowski (Luboń and Tarkowski 2020) analyzes shorter initial filling periods and found that the best initial filling period would be 2 years. Therefore, the presented article includes a 2-year period and longer ones – 3 and 4 years. By trial and error, the flow rates of the injected hydrogen were adjusted to the allowable pressures, so that the pressure in the top of the storage (i.e., in the roof section of the near-well zone and at the top of the structure) did not exceed the sum of the initial pressure and the caprock capillary pressure. When the pressure dropped by 0.1 MPa, we could increase the flow rate, but again, assuming that the pressure did not exceed the sum of the initial pressure and the caprock capillary pressure. These steps are repeated until the end of a 2, 3 or 4 year injection simulation. In this way, the variable hydrogen flow rate for the entire injection period of 4, 3, and 2 years was determined. Simulation conducted in this way results from the limitation of the used program (PetraSim TOUGH2). This limitation

consisted of the fact that we can only set the flow of the injected fluid but cannot set the limit pressure. So the fulfillment of the condition of not exceeding the permissible pressures consisted in adjusting the flow rate. Values of the determined flow rates multiplied by the time of their occurrence allowed for the calculation of the amount of hydrogen injected in the initial filling period (total capacity). Subsequently, the weighted average flow rate was determined. The weight in the calculation was the time of occurrence of a given flow rate, and the sum of the weights was equal to 1. The time-weighted average flow rate calculated in this way was used for the six-month hydrogen withdrawal period and thus allowed to calculate the amount of working gas. This working gas value was used to further 30-year cyclical withdrawal and injection.

Simulation of the UHS operation (injection and withdrawal). The next stage of work concerned the simulation of 30 operation cycles of UHS, in which an amount of hydrogen, defined as working gas, was injected and withdrawn at six-month intervals. During each hydrogen withdrawal cycle, deep saline aquifer water was also extracted. The difference between total capacity and working gas is the cushion gas capacity (cushion gas for six months, hydrogen withdrawal time period).

3. Results

3.1. Geological model of the Konary deep saline aquifer structure (trap)

It was assumed that the elliptical-oval outline of the anticline determines the isohypses of the Lower Pliensbach Jurassic roof, with a value of $-1,000$ m. The model's boundary was determined to cover the entire structure of this isohypse, reaching the fault near the structure. Based on these assumptions, the modeled area was around 92 km^2 . The area defined by the outline of the structure was determined by the isohypse $-1,000$ m (roof of the Komorowo Formation) and was approx. 48 km^2 . The number of computational cells in the PetraSim TOUGH2 spatial model in the geological structure of Konary was around 20,000 (Figure 1). The grid cells have an area of approximately $100,000 \text{ m}^2$. In addition, the grid was refined in the area of the structure boundary to an area of approximately $10,000 \text{ m}^2$, and in the area of the injection/withdrawal well to an area of approximately $1,000 \text{ m}^2$.

Model boundaries in the TOUGH2 modeling software are closed. However, by giving the border cells of the grid a very large volume (about 10^{50} m^3), these borders can be seemingly “infinite” (Pruess et al. 1999), which was done during the creation of the Konary structure model. Because in the vicinity of the Konary structure (at the model boundary Figure 1 red dashed line) there is probably a fault, the boundary has been closed in the place of its occurrence, as it may cause a faster increase in pressure that may exceed the allowable levels (Lothe et al. 2014) according to the authors' previous results on CO_2 injection (Luboń 2020, 2022).

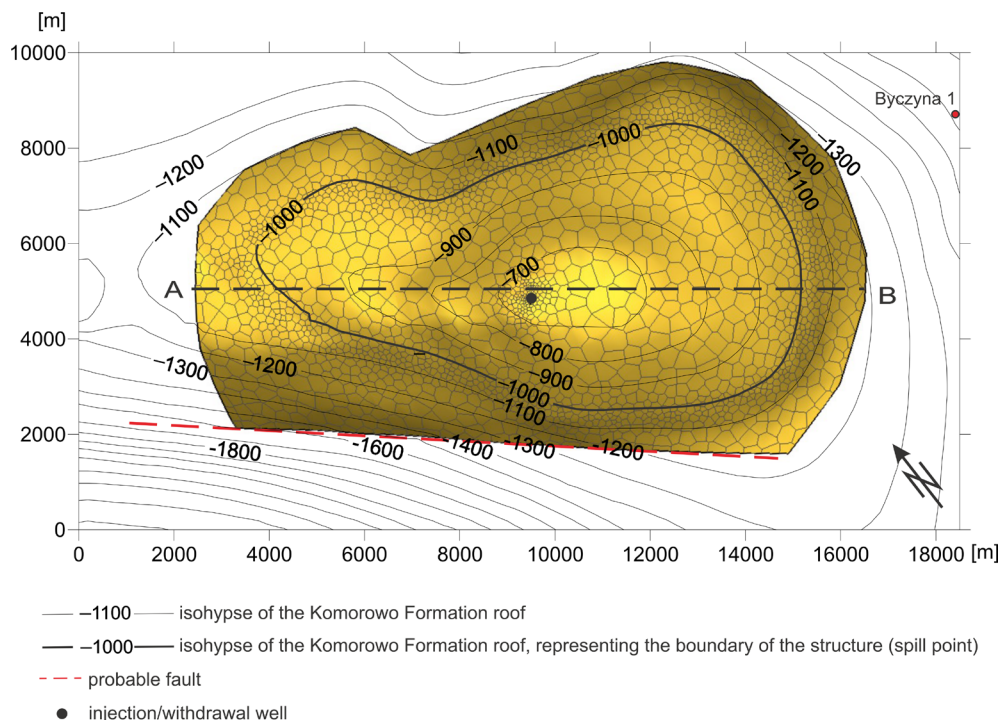


Fig. 1. Top-down view of Konary structure numerical model (based on Luboń 2022)

Rys. 1. Widok z góry modelu numerycznego struktury Konary

3.2. Allowable pressures: minimal fracturing pressure and caprock capillary pressure

Initial pressure was determined based on the pressure gradient, and its range is 7.4–8.21 MPa (for the roof and floor of this level, respectively) due to the fact that the thickness of the reservoir is almost 100 m. The minimal fracturing pressure was calculated for each of the ten selected layers, and therefore the range of it is 13.86–14.95 MPa in the roof and floor of the reservoir (Table 1).

The pore radius was adopted based on the results obtained by Tarkowski and Wdowin (Tarkowski and Wdowin 2011) and Tarkowski et al. (Tarkowski et al. 2014). The petrographic analysis of the pore space distribution of the Lower Jurassic caprock made it possible to determine the pore size to be 0.1–0.01 μm in diameter. For safety reasons, a pore diameter of 0.1 μm was used for the calculations. The calculated value of the caprock capillary pressure is 1.49 MPa, while the sum of the caprock capillary pressure and initial pressure in the reservoir roof is 9.25 MPa. This was taken as the limit value determining the hydrogen injection flow rate of the reservoir roof.

3.3. Simulation of hydrogen injection into the structure in three variants: 4, 3 and 2 years of the initial injection period

The upper part of Figure 2 shows the course of pressure during the initial filling of hydrogen into the Konary structure (blue, green and yellow lines). The allowable caprock capillary pressure, which is 9.25 MPa, is marked in red, and the pressure that is lower by 0.1 MPa (9.15 MPa) is marked with the red dashed line. The figure shows that the pressure in the initial phase of injection (in the first few days) increases rapidly. The pressure then fluctuates within the range of 9.15–9.25 MPa (i.e. in the range of 0.1 MPa adopted by the authors), as a result of adjusting the flow rate. In this way, the variable hydrogen flow rate for the entire injection period of 4, 3, and 2 years was determined (the lower part of Figure 2). Based on these variables flow rates, the total hydrogen capacity was calculated for each of the mentioned initial filling periods of 4, 3, and 2 years.

As a result of the hydrogen injection simulations in relation to the 4, 3, and 2 years initial filling periods, a time-weighted average value of the hydrogen flow rate of 1.17 kg/s was obtained.

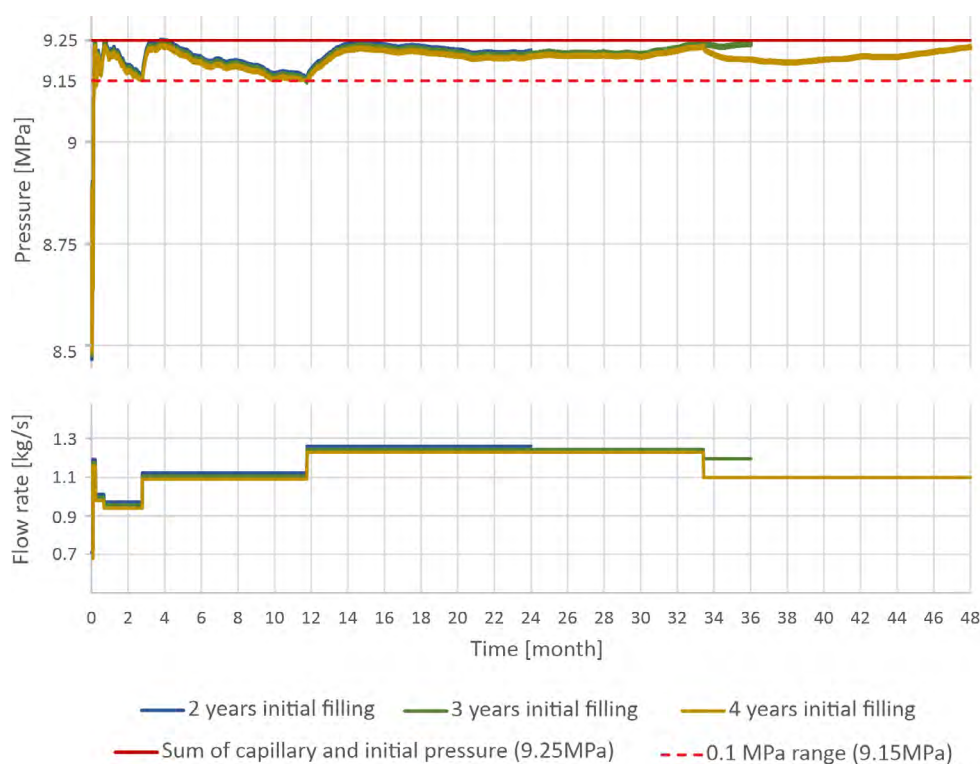


Fig. 2. The flow rate of the initial filling of hydrogen, adjusted to the pressure range

Rys. 2. Zakres ciśnień do którego dostosowany został przepływ wodoru
w okresie pierwszego napełniania magazynu wodorem

3.4. Simulation of the operation (injection and withdrawal) of UHS

The amount of working gas was calculated on the basis of the determined average flow rate, which is 1.17 kg/s, applied to the six-month hydrogen withdrawal period. Its value is 18,531 Mg. With this amount of working gas, the storage was operated for thirty cycles (six-month hydrogen injection and six-month hydrogen withdrawal). During each hydrogen withdrawal cycle, deep saline aquifer water was also extracted. Figure 3 shows the quantities of hydrogen injected and withdrawn (working gas) and the amount of water extracted, in each of the thirty injection and withdrawal cycles, for the option of a 4 year period of initial filling of the storage. Similar simulations of the thirty operation cycles of the hydrogen storage were performed for the remaining options of 3 and 2 year initial filling periods (Figure 4 and Figure 5).

Based on the simulations of initial filling with variable hydrogen flow rate, the total capacity was calculated, which is higher when the initial filling period is extended: over a period of 4 years, it would be 147,453 Mg, over 3 years – 112,650 Mg and over 2 years – 73,543 Mg (Table 2 and Figure 6).

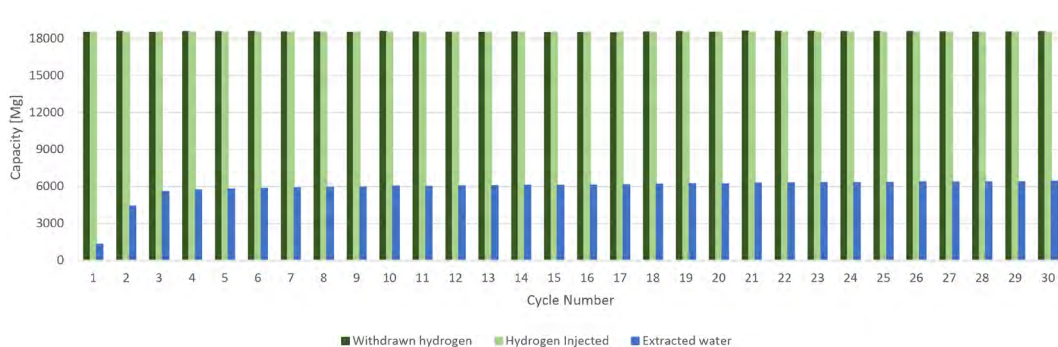


Fig. 3. Cyclical operation of hydrogen storage after 4 years of initial filling

Rys. 3. Cykliczna eksploatacja magazynu wodoru po pierwszym napełnieniu wynoszącym 4 lata

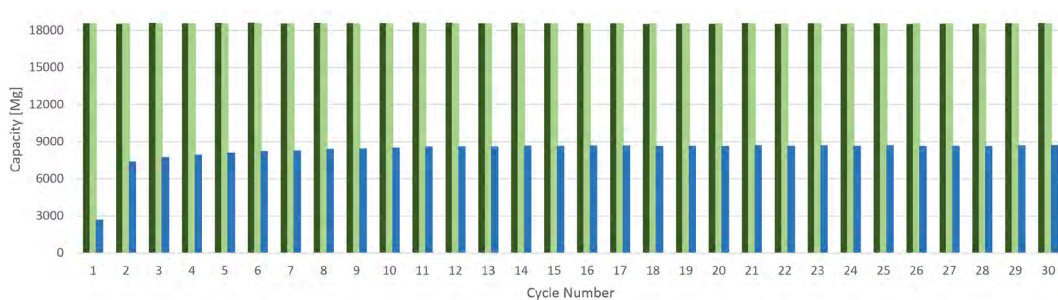


Fig. 4. Cyclical operation of hydrogen storage after 3 years of initial filling (color explanation as in Figure 3)

Rys. 4. Cykliczna eksploatacja magazynu wodoru po pierwszym napełnieniu wynoszącym 3 lata
(objaśnienie kolorów jak na rysunku 3)

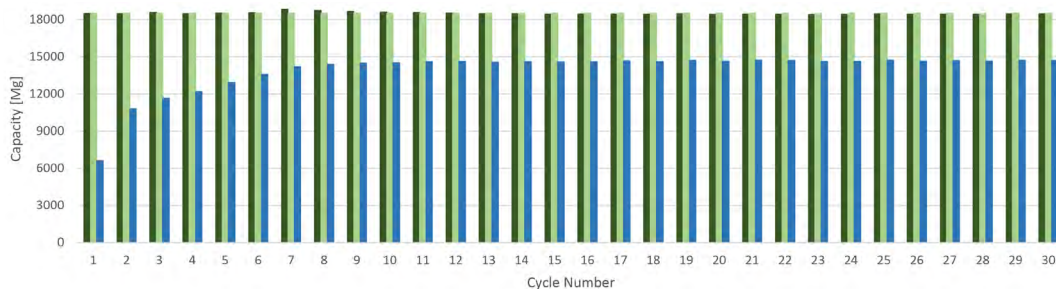


Fig. 5. Cyclical operation of hydrogen storage after 2 years of initial filling (color explanation as in Figure 3)

Rys. 5. Cykliczna eksploatacja magazynu wodoru po pierwszym napełnieniu wynoszącym 2 lata (objaśnienie kolorów jak na rysunku 3)

It was assumed that the amount of working gas would be the same regardless of the initial filling length. Therefore, for all initial hydrogen filling options, the amount of cushion gas over a six-month hydrogen withdrawal period would be variable. Over 4 years of initial filling, this would be 128,922 Mg, just over 87% of the total capacity, over 3 years, the figure would be 94,120 Mg (84% of the total capacity) and over 2 years – 55,012 Mg (almost 75% of the total capacity) (Table 2 and Figure 6).

The amount of extracted water during every cycle of hydrogen injection and withdrawal would less with a more extensive cushion gas capacity. Therefore, the amount of extracted water would increase as the initial filling period is shortened; over a 4 years of initial filling,

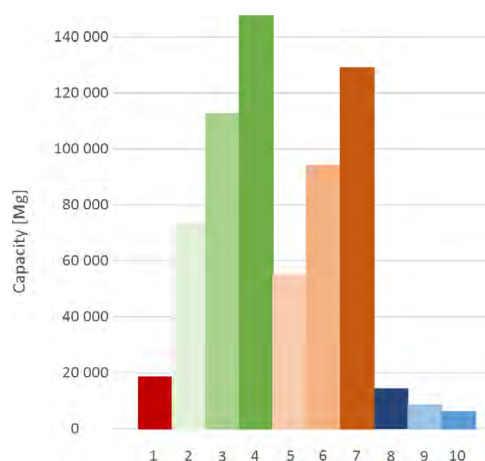


Fig. 6. Graph showing the comparison of the total capacity, cushion gas and extracted water for the considered cases of 2, 3 and 4 years of initial filling (numbers 1–10 correspond to those marked in grey in Table 2)

Rys. 6. Wykres przedstawiający porównanie pojemności całkowitej, poduszki gazowej i wyeksploatowanej wody dla rozpatrywanych przypadków 2-, 3- i 4-letniego okresu pierwszego napełniania (numery 1–10 odpowiadają tym zaznaczonym na szaro w tabeli 2)

Table 2. Characterization of hydrogen storage in the structure of Konary for the considered periods of 4, 3 and 2 years of initial filling (numbers 1–10 marked in grey in table correspond to x axis in Figure 6)

Tabela 2. Charakterystyka magazynu wodoru w strukturze Konary dla rozważanego 4-, 3- i dwuletniego okresu pierwszego napełniania (numery 1–10 zaznaczone na szaro w tabeli odpowiadają numerom na rys. 6 znajdującym się na osi x)

The initial filling period option	4 years	3 years	2 years	Unit
Amount of hydrogen injected during the initial filling (total capacity)	4	3	2	(Mg)
	147,453	112,650	73,543	
Working gas for six months of hydrogen withdrawal	1			
	18,533			
Cushion gas for six months of hydrogen withdrawal	7	6	5	
	128,922	94,120	55,012	
Average amount of extracted water during every cycle of hydrogen injection and withdrawal	10	9	8	
	6,145	8,525	14,421	
Total amount of extracted water during the thirty cycles of hydrogen injection and withdrawal	177,183	247,923	418,406	
Every cycle extracted water to working gas ratio	31.91%	46.95%	78.79%	
Cushion gas to total capacity ratio	87.43%	83.55%	74.80%	
Cushion gas to working gas (CG/WG) ratio	6.96	5.08	2.97	

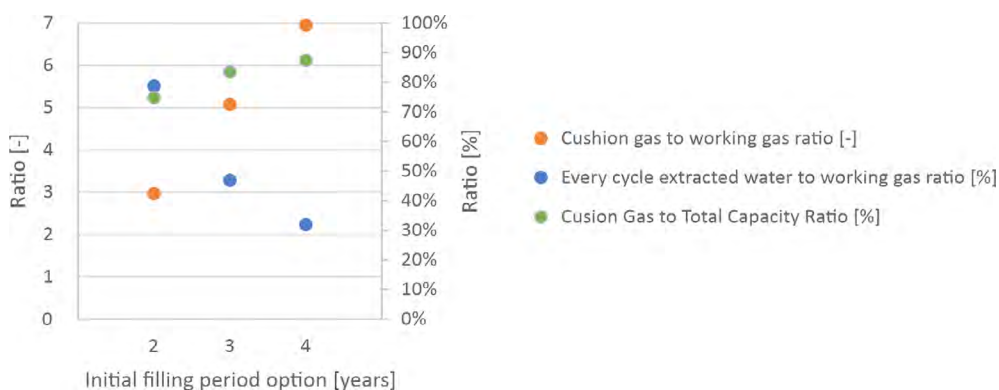


Fig. 7. Graph showing the comparison of ratios: every cycle extracted water to working gas, cushion gas to total capacity and cushion gas to working gas

Rys. 7. Wykres przedstawiający porównanie współczynników: woda eksploatowana w każdym cyklu do gazu roboczego, poduszka gazowa do pojemności całkowitej oraz poduszka gazowa do gazu roboczego

the amount of water extracted would be the lowest and amounts to 6,145 Mg and over 2 years, the amount would be the greatest, totaling 14,421 Mg (Table 2 and Figure 6). The same applies to the total amount of water that would be extracted during the thirty cycles of the storage operation. Throughout the initial filling period of 4 years, 177,183 Mg would be extracted, over 3 years, this figure would be 247,923 Mg and over 2 years – 418,406 Mg.

The results of the obtained simulations and calculations enabled the determination of every cycle of extracted water to working gas ratio. It varies in the range of 32–79% and decreases with the extension of the initial filling period. The cushion gas to total capacity ratio is 75–87% and also increases with the lengthening of the initial filling period. The cushion gas to working gas (CG/WG) ratio in our analysis ranges from 2.97 to 6.96 and significantly increases with the extension of the initial filling (Table 2 and Figure 7).

4. Discussion

The conducted research made it possible to determine the conditions for the preparation and operation of underground hydrogen storage of the Konary geological structure in Poland, previously identified for underground CO₂ storage (Luboń 2020, 2022). The simulations made it possible to determine the essential parameters affecting the underground hydrogen storage operation: maximum flow rate of injected hydrogen, total capacity, working gas capacity, and cushion gas capacity.

The results of research conducted by Sainz-Garcia et al. (Sainz-Garcia et al. 2017) demonstrate that the maximum hydrogen recovery ratio is 78%. Bai et al. (Bai et al. 2014) reported that under the same conditions, the required cushion gas for storage of hydrogen in a depleted oil and gas reservoir is 33% and for the storage of methane, it is 50%. Moreover, on the other hand, 33–66% and 80% are reported for hydrogen and methane storage in an aquifer, respectively. Muhammed et al. (Muhammed et al. 2023) report that the required of cushion gas for hydrogen storage in the deep saline aquifer is within the range of 33–80%, in salt cavern 20–33% and in depleted oil and gas 50–60%. Our research for the geological structure of Konary, using the three options of the initial filling periods of hydrogen storage, shows that the cushion gas needed is between 75 and 87%. The limit value is about 80% for the operation of hydrogen storage without excessive water extraction. These are large amounts of hydrogen, which are not working gas and will remain within the structure during the operation of the underground storage as cushion gas.

As shown in the present article, in addition to the withdrawal of hydrogen from its storage in the aquifer, the extraction of large amounts of water is a problem. This issue is highlighted by Harati et al. (Harati et al. 2023), who suggest that the extracted water be injected back into the reservoir. This problem is apparent when we operate the storage with one well used for injecting and withdrawing hydrogen, as assumed in the present article. The water extraction during hydrogen withdrawal from storage is also indicated by Ershadnia et al. (Ershadnia et al. 2022). It is worth remembering, however, that with an increase in the

size of the cushion gas the amount of water that is extracted during hydrogen withdrawal decreases. It should be noted that The EOS5 module of PetraSimTOUGH2 uses water, not brine, which may affect the water production rate. Taking into account the density difference between water and brine, the simulation results may have an error of 1.5–2%. This is a limitation of our research due to the capabilities of the available modeling software. Finally, due to the high cost of hydrogen production, it is most important for the authors to have as low level of cushion gas as possible. Water disposal will be an economic problem of much less importance.

Pressure changes observed during hydrogen injection into the aquifer structure determine the permissible injection rate. Pfeiffer and Bauer (Pfeiffer and Bauer 2019) evaluated the usefulness of simulation models to assess the rate of gas flow in the well and pressure changes. Okoroafor et al. (Okoroafor et al. 2022) also used simulations of hydrogen storage to analyze the injection scenario. They have demonstrated that numerical simulation is valuable for understanding the dynamics associated with hydrogen storage in depleted reservoirs and is useful for determining the optimal conditions for maximizing hydrogen withdrawal from storage sites.

Due to the costs of hydrogen that we have to incur when preparing underground storage for operation, the best option for hydrogen storage seems to be the shortest, namely, 2 years of initial hydrogen filling in the structure – this is the option with the least amount of cushion gas.

The obtained results refer to the storage of hydrogen in the geological structure of Konary, with a reservoir level at a depth of 700–1000 m. Related results should be obtained for similar structures located at similar depths. It would be interesting to recognize the possibility of hydrogen storage in the case of the same structure, with a reservoir at different depths, as shown for the Suliszewo structure (Luboń and Tarkowski 2023). From an economic point of view, hydrogen storage in porous media is associated with large losses of hydrogen as a cushion gas, and probably also as a result of partial diffusion into the caprock. For this reason, it seems that where there are salt deposits, salt caverns are more favorable places for hydrogen storage. On the other hand, porous structures provide much larger storage capacities and are an alternative in places where there are no salt deposits (Zivar et al. 2021; Muhammed et al. 2022; Hematpur et al. 2023).

Conclusions

The research is site specific and was intended to determine the conditions for the preparation and operation of UHS in Konary geological structure (trap). This was achieved by modeling the injection and withdrawal of hydrogen in the deep Lower Jurassic saline aquifer of the Konary structure. This type of research is essential when planning the use of the geological structure of the deep saline aquifer for UHS and allows us to determine the maximum flow rate of injected hydrogen and then the total capacity, the working gas

capacity, and the cushion gas capacity. The obtained results are relevant for the analysis of the underground hydrogen storage operation and affect the economic aspects of UHS in deep aquifers.

Due to the hydrogen costs we incur when preparing underground storage for operation, the best option for hydrogen storage seems to be the shortest of the three considered – the 2 year period of hydrogen initial filling in the structure and, consequently, the option with the least cushion gas.

The amount of water that is extracted during hydrogen withdrawal decreases with the increasing length of the initial hydrogen filling period. Extracted water poses a problem with regard to its disposal.

The results indicate hydrogen storage in a porous media geological structure at a specific depth. It would be interesting to explore the possibilities of storage at different depths. From an economic point of view, hydrogen storage in porous media provides a much larger storage capacity. It is an alternative to cavern storage in salt deposits, where much smaller amounts of cushion gas are required.

This work was supported by the Mineral and Energy Economy Research Institute of the Polish Academy of Sciences (research subvention).

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NUMERICAL SIMULATION OF HYDROGEN STORAGE IN THE KONARY DEEP SALINE AQUIFER TRAP

Keywords

underground hydrogen storage, deep saline aquifer,
numerical simulation, hydrogen injection and withdrawal

Abstract

Nowadays, hydrogen is considered a potential successor to the current fossil-fuel-based energy. Within a few years, it will be an essential energy carrier, and an economy based on hydrogen will require appropriate hydrogen storage systems. Due to their large capacity, underground geological structures (deep aquifers, depleted hydrocarbon fields, salt caverns) are being considered for hydrogen storage. Their use for this purpose requires an understanding of geological and reservoir conditions, including an analysis of the preparation and operation of underground hydrogen storage.

The results of hydrogen injection and withdrawal modeling in relation to the deep Lower Jurassic, saline aquifer of the Konary geological structure (trap) are presented in this paper. A geological model of the considered structure was built, allowable pressures were estimated, the time period of the initial hydrogen filling of the underground storage was determined and thirty cycles of underground storage operations (gas injection and withdrawal) were simulated. The simulations made it possible to determine the essential parameters affecting underground hydrogen storage operation: maximum flow rate of injected hydrogen, total capacity, working gas and cushion gas capacity. The best option for hydrogen storage is a two-year period of initial filling, using the least amount of cushion gas. Extracted water will pose a problem in relation to its disposal. The obtained results are essential for the analysis of underground hydrogen storage operations and affect the economic aspects of UHS in deep aquifers.

SYMULACJA NUMERYCZNA MAGAZYNOWANIA WODORU W GŁĘBOKIM SOLANKOWYM POZIOMIE WODONOŚNYM STRUKTURY KONARY

Słowa kluczowe

symulacja numeryczna, podziemne magazynowanie wodoru,
głębokie poziomy wodonośne, zatłaczanie i odbiór wodoru

Streszczenie

Ze względu na bardzo dużą pojemność podziemne struktury geologiczne (głębokie poziomy wodonośne, szczerpane złoża węglowodorów, kawerny solne) są rozważane do magazynowania wodoru. Ich wykorzystanie w tym celu wymaga rozpoznania uwarunkowań geologiczno-złożowych, w tym

analizy przygotowania oraz pracy podziemnego magazynu wodoru. Przedstawiono wyniki modelowania zatłaczania i odbioru wodoru do głębokiego dolnojurajskiego poziomu solankowego struktury geologicznej Konary. Zbudowano model geologiczny rozważanej struktury, oszacowano dopuszczalne ciśnienia szczelinowania oraz ciśnienie kapilarne nadkładu, wyznaczono długości wstępnego okresu zatłaczania wodoru do podziemnego magazynu, przeprowadzono modelowanie przebiegu 30-letniej pracy podziemnego magazynu (zatłaczania i odbioru gazu). Przeprowadzone symulacje umożliwiły określenie istotnych parametrów wpływających na prace podziemnego magazynu wodoru: maksymalną wielkość przepływu zatłaczanego wodoru, pojemność całkowitą, pojemność roboczą i wielkość poduszki gazowej. Pozwoliły stwierdzić, że im dłuższy wstępny okres zatłaczania wodoru, tym większą musimy zastosować poduszkę gazową. Za najlepszą opcję dla magazynowania wodoru zaproponowano dwuletni okres wstępnego zatłaczania gazu do struktury; opcja z najmniejszą wielkością poduszki gazowej. Stwierdzono, że ilość wody, jaka jest eksploatowana w trakcie odzyskiwania wodoru, podczas cyklicznej eksploatacji magazynu, spada wraz ze zwiększeniem długości wstępnego okresu zatłaczania wodoru. Eksploatowana woda będzie stanowiła znaczący problem związany z jej unieszkodliwieniem. Otrzymane wyniki są istotne w analizie pracy podziemnego magazynu wodoru i wpływają na aspekty ekonomiczne UHS w głębokich solankowych poziomach wodonośnych.