Nafta-Gaz 2021, no. 12, pp. 783-794, DOI: 10.18668/NG.2021.12.01

Numerical procedure to effectively assess sequestration capacity of geological structures

Numeryczna procedura efektywnego szacowania pojemności sekwestracyjnej struktur geologicznych

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ABSTRACT: The paper presents a numerical procedure of estimating the sequestration capacity of an underground geological structure as a potential sequestration site. The procedure adopts a reservoir simulation model of the structure and performs multiple simulation runs of the sequestration process on the model according to a pre-defined optimization scheme. It aims at finding the optimum injection schedule for existing and/or planned injection wells. Constraints to be met for identifying the sequestration capacity of the structure include a no-leakage operation for an elongated period of the sequestration performance that contains a relaxation phase in addition to the injection one. The leakage risk analysis includes three basic leakage pathways: leakage to the overburden of a storage formation, leakage beyond the structural trap boundary, leakage via induced fractures. The procedure is implemented as a dedicated script of the broadly used Petrel package and tested on an example of a synthetic geologic structure. The script performs all the tasks of the procedure flowchart including: input data definitions, simulation model initialization, iteration loops control, simulation launching, simulation results processing and analysis. Results of the procedure are discussed in detail with focus put on various leakage mechanisms and their handling in the adopted scheme. The overall results of the proposed procedure seem to confirm its usefulness and effectiveness as a numerical tool to facilitate estimation of the sequestration capacity of an underground geological structure. In addition, by studying details of the procedure runs and its intermediate results, it may be also very useful for the estimation of various leakage risks.

Key words: CO₂ sequestration, reservoir modelling, numerical simulations, multiphase migration, leakage pathways.

STRESZCZENIE: W artykule przedstawiono numeryczną procedurę szacowania pojemności sekwestracyjnej podziemnej struktury geologicznej jako potencjalnego obiektu sekwestracji. Procedura wykorzystuje symulacyjny model złożowy struktury i wykonuje wielokrotne przebiegi symulacyjne procesu sekwestracji na jej modelu zgodnie ze skonstruowanym w ramach pracy schematem optymalizacyjnym. Jego celem jest znalezienie optymalnego programu zatłaczania sekwestrowanego CO₂ za pomocą istniejących i/lub planowanych odwiertów zatłaczających. Warunkiem koniecznym określenia pojemności sekwestracyjnej struktury jest brak ucieczki sekwestrowanego gazu w zakładanym okresie funkcjonowania obiektu, obejmującym wieloletnią fazę relaksacji po zakończeniu właściwego etapu zatłaczania. Analiza ryzyka ucieczki sekwestrowanego gazu rozpatruje trzy podstawowe drogi ucieczki: do nadkładu formacji składowania, poza granicę pułapki strukturalnej, przez indukowane szczeliny lub inne elementy nieciągłości struktury. Procedura ta zaimplementowana jest jako skrypt szeroko stosowanego pakietu Petrel firmy Schlumberger i testowana jest na przykładzie syntetycznej struktury geologicznej przedstawiającej fragment antykliny. Do opisu modelu statycznego oraz dynamicznego wykorzystano parametry pochodzące z modelu struktury, do której obecnie zatłaczane są powrotnie gazy kwaśne. Skrypt ten realizuje wszystkie zadania schematu blokowego procedury, obejmujące: definiowanie danych wejściowych, inicjowanie modelu symulacyjnego, sterowanie pętlami iteracji, uruchamianie symulacji, przetwarzanie i analizę wyników symulacji. Szczegółowo omówione zostały wyniki procedury, z uwzględnieniem różnych mechanizmów ucieczki, i ich analiza w przyjętym schemacie. Ogólne wyniki proponowanej procedury potwierdzają jej przydatność i skuteczność jako narzędzia numerycznego do oceny pojemności sekwestracyjnej podziemnych struktur geologicznych. Ponadto, poprzez badanie szczegółów przebiegu procedury i jej pośrednich wyników wskazuje, że narzędzie to może być również bardzo przydatne do szacowania różnych zagrożeń ucieczki sekwestrowanego gazu z badanej struktury.

Słowa kluczowe: sekwestracja CO₂, modelowanie złożowe, symulacje numeryczne, migracja wielofazowa, typy ucieczki sekwestrowanego gazu.

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Article contributed to the Editor: 06.10.2021. Approved for publication: 30.11.2021

Introduction

The idea of CO₂ injection into subsurface geological structures for its sequestration is widely used (Lubaś and Stopa, 1997; Lubaś and Szott, 2010; Lubaś et al., 2012; Polish Oil and Gas Company, 2019). This process is determined to much extent by the effects of injected gas migration within the structure and beyond its borders (Qi and Guizhen, 2015) which leads to the leakage of the gas (Mathieson et al., 2011). The most likely migration routes are: overburden rocks (Sorai et al., 2014; Roberts et al., 2017), barriers/faults, fractures (Alexander and Boodlal 2014; Yang et al., 2018), zones along well trajectories (Brydie et al., 2014; Doherty et al., 2017) and escaping beyond structural trap boundaries (Zhang et al., 2017; Zapata et al., 2020). Substantial simulation models (which combine all types of data defining a hydrocarbon reservoir) are of significant help in analysing migration of the injected CO₂ (Szott et al., 2009; Khan et al., 2013; Mackay, 2013; Nakajima et al., 2014; Diao et al., 2020; Zapata et al., 2020).

An appropriate procedure supported by numerical analysis of simulation results allows to determine the sequestration capacities of analysed structures. For these purposes, it is possible to apply an automatic procedure implemented in a computer algorithm in the form of a script (workflow) that controls operation of the appropriate software tool (Petrel, 2020). The use of simulation results and the automation of the process of generating subsequent prognostic scenarios effectively reduces the number of simulations needed for the analysis and thus the time needed for their execution.

Currently, workflow schemes, initially used only for the construction of geological models, are becoming more and more popular in the field of reservoir simulations, and the increasing possibilities of their use confirm their high utility in this field.

The aim of this study is to determine the sequestration capacity of the analysed structure using the above-mentioned Petrel package development tool. This procedure was performed on a synthetic model showing a fragment of the anticline. To describe the static and dynamic models, the parameters derived from the model of the structure to which acid gases are currently re-injected were used (Lubaś et al., 2020).

The work uses the Petrel package (Petrel, 2020) together with the Eclipse 300 reservoir simulator (Eclipse Black Oil and Compositional, 2010) by Schlumberger.

Model of a synthetic reservoir

General characteristics of migration effects in a 3D model

In order to simulate the CO_2 sequestration process and assess the sequestration capacity, a three-dimensional synthetic

model was used. This model is made of 9620 active blocks that form a segment – a quarter of the regular anticline. Each single simulation block measures 50×50 m in lateral directions and 5 m of height. The grid consists of $31 \times 31 \times 20$ homogeneous blocks characterized by uniform porosity and permeability in the reservoir zone and limited permeability of the overburden represented by the first model layer (k = 1). The study uses a homogeneous model to focus on other significant aspects (no-leakage criteria) of the simulation of the sequestration processes and assumes a limited significance of heterogeneity on such simulation results (Szott et al., 2009). The model view is shown in Figure 1. Its upper part is assumed to be filled with CO₂ (Fig. 2) as a result of initial injection, which increases the formation pressure, P_{ini} from 149 to 156 bar.





Fig. 1. 3D view of a gas reservoir synthetic model Rys. 1. Widok 3D modelu syntetycznego złoża gazu



Fig. 2. Initial gas saturation distribution. Reservoir layers only (k = 2 - 20)

Rys. 2. Początkowy rozkład nasycenia gazem (przed dotłaczaniem gazu). Widok bez nadkładu (dla k = 2 - 20)

artykuły

Gas leakage to overburden

Gas leakage from the reservoir to its overburden is determined by the reservoir-caprock threshold pressure. The value of this pressure is adopted from a realistic case and amounts to $P_{th} = 9.9$ bar, and refers to the maximum pressure difference (between the reservoir top and caprock bottom) that ensures caprock tightness. The distribution of the reservoir pressure (Fig. 3) after the initial injection phase guarantees the tightness of the caprock.

Pressure [bar]



Fig. 3. Initial pressure distribution. Overburden layer, k = 1, reservoir layers, k = 2 - 20

Rys. 3. Ciśnienie początkowe (przed dotłaczaniem gazu) w nadkładzie (k = 1) oraz w złożu (k = 2 - 20)

Gas leakage beyond the structural trap boundary

In order to model the escape beyond the boundary of the reservoir trap, this boundary is defined as the gas–water contact contour on the top of the reservoir (Fig. 4).

Gas leakage via induced fractures

The dynamic model assumes the formation breakdown (fracturing) pressure to be $P_{frac} = 1.25 \times P_{ini} = 186$ bar. In order to eliminate the risk of leakage through the induced fractures, instructions are implemented in the procedure to prevent the maximum reservoir pressure around the injection wells from exceeding the fracturing pressure.

General assumptions of the simulation procedure

Basic assumptions of the CO₂ sequestration project:

- duration of the injection phase, $t_{inj} = 2$ years;
- hydrostatic pressure distribution in the overburden;
- 3 injection wells located at the top of the reservoir structure (Fig. 1).



Fig. 4. Definition of regions for the leakage beyond the structural trap boundary of the reservoir: region no. 1 -external zone, region no. 2 -internal zone. View of reservoir layers only (k = 2 - 20)

Rys. 4. Definicja regionów dla kryterium ucieczki poza granice złoża. Region 1 – strefa poza konturem gaz–woda, Region 2 – strefa wewnątrz konturu gaz–woda. Widok bez nadkładu (k = 2 - 20)

Procedure of maximum injection with no-leakage criteria

No-leakage criteria

The reservoir model described above is supplemented with additional elements necessary to estimate (maximize) the amount of injected CO_2 .

The following criteria are used to ensure a no-leakage injection:

- 1) tightness of the caprock: pressure step, ΔP , across the reservoir-caprock boundary does not exceed the threshold pressure of the caprock, $\Delta P \leq P_{th}$;
- 2) no leakage beyond the structural trap boundary;
- 3) no leakage through to induced fractures.

Procedure to determine sequestration capacity

Based on the above criteria, the algorithm of proposed procedures is described in the flowchart presented in Figure 5.

The algorithm consists of 3 key nested components (from the most inner to the most outer):

- simulation performance of the complete sequestration project;
- iterative optimization of the distribution of the total injected CO₂ stream among individual wells to satisfy a leakage-free sequestration process – inner loop;



Fig. 5. Flowchart of the algorithm to determine the sequestration capacityRys. 5. Schemat blokowy dla algorytmu wyznaczania pojemności sekwestracyjnej

3) iterative optimization of the total injected CO₂ to maximize the sequestration volume – outer loop.

This procedure is used to create the code in the scripting language (workflow) of the Petrel ver. 2020, the first part of which is shown in Figure 6 below.

In the above part, the following lines define, among others:

- lines 2–4 factors scaling the shares of injection wells I1, I2, I3 for the initial iteration, \$MGRI1, \$MGRI2, \$MGRI3;
- line 5 identification of the well responsible for the leakage – subjected to the reduction of its injection fraction, \$w (in the initial iteration \$w = 0 – no scaling of the injection fraction for any of the wells);
- line 6 total injection rate for the initial iteration, \$Ginj;
- line 7 threshold pressure, \$prog;
- line 8 maximum allowed gas leakage beyond the structural trap boundary, \$Vuclim (Fig. 4), above which the program performs subsequent steps to limit the leakage;
- line 9 multiplicative factor reducing the well injection rate, \$RedUO;
- line 10 multiplicative factor reducing the total injection rate \$RedGinj;
- line 11 initialization of the internal iteration counter, \$i;
- line 12 maximum number of internal iterations, \$imax;
- line 13 initialization of the outer iteration counter, \$j;
- line 14 maximum number of external iterations, \$jmax;
- line 15 the call of procedures to initialize the numerical simulation and to launch the simulation.

Later in the script, there are instructions in loops that operate on distributions of reservoir quantities (pressure, saturations) that result from iterative simulations. Based on the calculated values, in each subsequent iteration, the contribution of the well responsible for gas leakage is modified or the total injection rate is limited.

For each of the simulations defined by the script, a condition is attached to eliminate the possibility of gas leakage through the induced fracture as a result of exceeding the fracturing pressure.

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Injection optimization for the leakage criteria

Three groups of simulations called options were studied as presented below.

Option I – assumptions

Based on the script described above, the procedure of estimating the sequestration capacity of the analyzed structure was carried out. For the first option of maximizing this quantity, the following parameters were adopted:

- initial total injection rate, $Ginj = 30\ 000\ Sm^3/d;$
- initial injection rates of individual wells: GR I1 = GR I2 = = GR I3 = 33.33% of \$Ginj;
- threshold pressure, \$prog = 9.9 bar;
- maximum, allowed gas leakage beyond the trap boundary, \$Vuclim = 1 Rm³;
- multiplicative factor to reduce the contribution of a well to the total injection, \$RedUO = 0.85, multiplicative factor reducing the total injection rate, \$RedGinj = 0.9;
- maximum number of internal iterations, \$imax = 4;
- maximum number of external iterations, \$jmax = 100.

Option I – results

As a result of the sequestration capacity estimation procedure, the program generated 33 simulations. Their results in the form of total injection rates are shown in Figure 7. Each visible curve in the figure represents one external iteration consisting of four internal iterations (one iteration with the initial injection rates for the wells + three iterations with reduced rates of the wells).

The exception is the last external iteration for which the procedure has been completed after the first internal iteration due to the fulfilment of all the criteria for no CO_2 leakage outside the structure.

As a result of the procedure, the sequestration volume, for which there was no gas leakage into the overburden, beyond the reservoir trap and through the fracture, was estimated.

> It was found to be, $V_{sekwCO_2} = 618.4 \times 10^6 \text{ Sm}^3$ (Fig. 8) at \$Ginj = 12914 Sm³/d. As for the total injection of 619.6 × 10⁶ Sm³, the leakage of CO₂ was observed; the relative error of the sequestration volume was estimated not to exceed 0.19%.

Option II – assumptions

Since for Option I no leakage beyond the boundaries of the reservoir or via induced fractures was observed, for comparison purpose Option II of the procedure was performed characterized by an increased initial



Fig. 7. Scenarios of Option I. CO₂ injection rate **Rys. 7.** Wariant I. Sumaryczna wydajność zatłaczania CO₂

Fig. 8. Scenarios of Option I. Sequestration capacity for subsequent iterations

Rys. 8. Wariant I. Pojemność sekwestracyjna dla kolejnych iteracji

total injection rate and those of individual wells with the exception of I3 well located on the edge of the model and affected by a smaller area compared to the remaining wells. Below are the process parameters used for Option II:

- initial total injection rate, $Ginj = 100\,000\,Sm^3/d$;
- initial injection of individual wells: GRI1 = GRI2 = 44.44%, GRI3 = 11.11% of \$Ginj;
- threshold pressure, \$prog = 9.9 bar (as in Option I);
- maximum, allowed gas leaage beyond the trap boundary, \$Vuclim = 1 Rm³ (as in Option I);
- multiplicative factor to reduce the contribution of a well to the total injection, \$RedUO = 0.5;
- multiplicative factor to reduce the total injection rate, \$RedGinj = 0.5;
- maximum number of internal iterations, \$imax = 3 (as in Option I);
- maximum number of external iterations, \$jmax = 100 (as in Option I).

Option II – results

As a result of the sequestration capacity estimation procedure carried out in Option II, the program generated 13 simulations. The results in the form of total injection rates are shown in Figure 9. Each visible curve in the figure represents one external iteration of four internal iterations (one iteration with initial injection rates for the wells + three iterations with reduced rates for wells).

As in Option I, the exception is the last external iteration for which the procedure has been completed after the first internal iteration due to the fulfilment of all the criteria for no CO_2 leakage outside the structure. Because for the simulations carried out in the first external iteration with the total injection rate, $Ginj = 1.0 \times 10^5 \text{ Sm}^3/\text{d}$ fracturing pressure was exceeded, the corresponding I3 well was closed before the injection process was completed while the rates of the remaining boreholes were increased in order to maintain a constant total injection rate. About 1.5 months after the shutdown of the I3 well,



Fig. 9. Scenarios of Option II. CO₂ injection rate **Rys. 9.** Wariant II. Sumaryczna wydajność zatłaczania CO₂

Fig. 10. Scenarios of Option II. Sequestration capacity for subsequent iterations Rys. 10. Wariant II. Pojemność sekwestracyjna dla kolejnych iteracji

the remaining wells, i.e. I1 and I2, were also closed for the same reason.

For Option II, the estimated sequestration volume was, $V_{sekwCO_2} = 617.1 \times 10^6 \text{ Sm}^3 \text{ at } \text{\$Ginj} = 12.5 \times 10^3 \text{ Sm}^3/\text{d.}$

As for the total injection of 626.2×10^6 Sm³, the leakage of CO₂ was observed; the relative error of the sequestration volume was estimated not to exceed 1.48%.

Option III – assumptions

Because a relatively high error of sequestration capacity was obtained for Option II, the procedure of estimating this value was repeated in Option III, where parameters influencing the convergence of the process were modified. The process parameters used for Option III are as follows:

- initial total injection rate, $Ginj = 1.0 \times 10^5 \text{ Sm}^3/\text{d};$
- initial injections of the individual wells: GRI1 = GRI2 = = 44.44%, GRI3 = 11.11% of \$Ginj;
- threshold pressure, \$prog = 9.9 bar (as in Options I and II);

- maximum, allowed gas leakage beyond the trap boundary, \$Vuclim = 1 Rm³;
- multiplicative factor to reduce the contribution of a well to the total injection, \$RedUO = 0.8;
- multiplicative factor to reduce the total injection rate, \$RedGinj = 0.8;
- maximum number of internal iterations, \$imax = 5;
- maximum number of external iterations, \$jmax = 100 (as in Options I and II).

Option III – results

As a result of the sequestration capacity estimation procedure carried out in Option III, the program generated 61 simulations. The results in the form of cumulative injection rates are shown in Figure 11. Each visible curve in the figure represents one external iteration composed of six internal iterations (one iteration with the initial injection rates for the wells + five simulations with reduced contributions).



Fig. 11. Scenarios of Option III. CO₂ injection rate **Rys. 11.** Wariant I. Sumaryczna wydajność zatłaczania CO₂

Fig. 12. Scenarios of Option III. Sequestration capacity for subsequent iterationsRys. 12. Wariant III. Pojemność sekwestracyjna dla

As in the previous cases, the exception is the last external iteration for which the procedure has been completed after the first internal iteration due to the fulfilment of all the criteria determining no CO_2 leakage out of the structure. Due to the higher value of the total injection reduction parameter (\$RedUO = 0.8), the shutdown mechanism for wells in which the fracturing pressure was exceeded took place in three external iterations. As in Option II, after the shutdown of the I3 well, the remaining wells had an increased rate to maintain a constant total injection rate.

For Option III, the estimated sequestration capacity is, $V_{sekwCO_2} = 615.77 \times 10^6 \text{ Sm}^3$ at \$Ginj = 10737 Sm³/d and the relative error of the sequestration capacity is found not to exceed 0.32%.

Detailed analysis of the procedure

The proposed procedure implemented in the form of a script in the Petrel package provides an opportunity to perform a detailed analysis of various procedure auxiliary and transitional results such as the location of leakage spots and effectiveness of their elimination with adopted remediation activities. The illustration of the procedure in action is described below.

In Option I, the only criterion effective in the iterative determination of the sequestration capacity is that of the threshold pressure across the reservoir-caprock boundary.

Consequently, the applied algorithm works as follows:

- a site (block) where the pressure step across the reservoircaprock boundary exceeds the threshold pressure is identified as the red block shown in Figure 13;
- the well responsible for that exceeding is identified by the highest contribution of the gas injected by that well and marked by a unique tracer (Fig. 14);
- the rate of gas injected by this well is reduced and the simulation of the injection process is repeated anew;
- the above steps are repeated until a no gas-leakage solution is achieved or the maximum, allowed number of internal



Fig. 13. Scenarios of Option I. Initial iteration. Pressure steps across the top boundary of the reservoir

Rys. 13. Wariant I. Iteracja początkowa. Różnica ciśnienia na stropie złoża oraz ciśnienia w nadkładzie

iterations is reached – otherwise, the total CO_2 injection into the reservoir is reduced and the next external iteration is carried out.

A modified initial, total injection rate in Options II and III results in an effective application of another no-leakage sequestration criterion (criterion no. 3 in the list of the Section "No-leakage criteria" above) concerning the fracturing pressure. Figure 15 shows the time evolution of pore pressures in model blocks completed by the CO_2 injecting the I3 well/by



Fig. 14. Scenarios of Option I. Initial iteration. The concentration of the tracer injected with the I3 well

Rys. 14. Wariant I. Iteracja początkowa. Koncentracja znacznika tłoczonego przez odwiert I3

 CO_2 being injected into the I3 well (red, solid lines) with rates given by the red, dashed line. As the maximum pressure exceeds the fracturing pressure, the injection rate of the well is reduced and, consequently, the next iteration (green, dashed line in Fig. 15) of the injection simulation run results in reduced pore pressures (green, solid lines in Fig. 15) and complies with the no-leakage process for the discussed criterion.



Fig. 15. Scenarios of Option II. Initial iteration (red lines): CO_2 injection rate of I3 well (dashed red line), pressure in blocks of I3 well completion (solid red lines); iteration with reduced injection rate (green lines) CO_2 injection rate of I3 well (dashed green line), pressure in blocks of I3 well completion (solid green lines)

Rys. 15. Wariant II. Iteracja początkowa (kolor czerwony) oraz iteracja ze zmniejszoną sumaryczną wydajnością zatłaczania (kolor zielony). Ciśnienie w blokach (linia ciągła) oraz wydajność zatłaczania CO₂ przez odwiert I3 (linia przerywana)

The case of criterion no. 2 in the list of the Section "No-leakage criteria" i.e. the leakage beyond the boundaries of the reservoir structural trap, is solved by checking against an increase of gas volume in the region external to the reservoir.

When such a change is identified and the leakage point is located (red block in Fig. 16) then concentrations of markers ascribed to all the individual wells are checked (Fig. 17, 18, 19) to find which well contributes to the leakage. Then the injection rate of the responsible well is reduced and the injection procedure is repeated. Otherwise, as for the described case where no well/none of the wells is found to directly contribute to the gas leakage across the boundary, the total injection rate for sub-





Fig. 16. Scenarios of Option II. Initial iteration. Change of gas volume in the external zone

Rys. 16. Wariant II. Iteracja początkowa. Zmiana objętości gazu poza obszarem złoża



Tracer concentration [-]

Fig. 17. Scenarios of Option II. Initial iteration. The concentration of the tracer injected with the II well

Rys. 17. Wariant II. Iteracja początkowa. Koncentracja znacznika tłoczonego przez odwiert I1

sequent iterations is reduced until the criterion of no-leakage beyond the boundaries of the reservoir structural trap is fulfilled.

As a result of the procedure of estimating the sequestration volume in Option I, $V_{sekwCO_2} = 618.4 \times 10^6 \text{ Sm}^3$ was obtained with an overestimation error below $1.7 \times 10^6 \text{ Sm}^3$. In subsequent Options, not only the parameters determining the convergence of the procedure were changed, but also the initial parameters, such as the total injection rate and the initial injection contributions of the individual wells. As a result, the estimated sequestration capacity was $V_{sekwCO_2} = 617.1$ and $615.8 \times 10^6 \text{ Sm}^3$ with errors below 9.1 and $1.9 \times 10^6 \text{ Sm}^3$ for Option II and Option III, respectively – Fig. 20.



Fig. 18. Scenarios of Option II. Initial iteration. The concentration of the tracer injected with the I2 well

Rys. 18. Wariant II. Iteracja początkowa. Koncentracja znacznika tłoczonego przez odwiert I2



Fig. 19. Scenarios of Option II. Initial iteration. The concentration of the tracer injected with the I3 well

Rys. 19. Wariant II. Iteracja początkowa. Koncentracja znacznika tłoczonego przez odwiert I3



Fig. 20. Sequestration capacity of various scenarios Rys. 20. Podsumowanie wyników szacowania pojemności sekwestracyjnej

It should be noted that the obtained values of the sequestration capacity in all three options are consistent with one another taking into account the limits of the error found to be 1.7, 9.1, and 1.9×10^6 Sm³ for Option I, II, and III, respectively.

Summary and conclusions

The paper presents a procedure of the automatic, computer performed estimation of the CO₂ sequestration capacity of a geologic structure. The procedure applies a numerical, reservoir simulation model of the structure and multiple simulations of the sequestration process on the model. The procedure takes advantage of a two-level iteration scheme to optimize the injection process by adjusting the total injection rate and its distribution among individual injection wells. The injection scheme is constrained by a standard schedule and technical assumptions and looks for a maximum injected volume without injected gas leakage of a three-way kind: (i) leakage to overburden, (ii) leakage beyond the structural trap boundary, (iii) leakage via induced fractures. It is worth noting that the procedure simulation forecasts include an elongated time for the relaxation phase of the sequestration projects – an issue important for the fulfilment of legal requirements.

The procedure is controlled by a dedicated script that is implemented as a "workflow" of the Petrel package by Schlumberger. The script performs all the tasks of the procedure flowchart including:

- 1) input data definitions;
- 2) simulation model initialization;
- 3) iteration loops control;
- 4) simulation launching;
- 5) simulation results' processing and analysis.

Results of the procedure operation are shown for an example of a synthetic geologic structure. They are discussed in detail with the focus put on various leakage mechanisms and their handling in the proposed procedure.

To conclude, it should be stated that the proposed procedure of estimating the sequestration capacity allows to effectively assess the value of this characteristic of a sequestration object. The negligible low dependence of the results on the initial conditions of the iterative procedure used confirms its practical value. In particular, the procedure may significantly facilitate the solution of problems related to the optimum selection of the operation parameters of sequestration projects, such as: the number of injection wells, total injection time, etc. By studying details of the procedure runs and, in particular, its intermediate results, it may be also very useful for the estimation of various leakage risks.

This paper was written on the basis of the statutory work entitled: *Efektywna ocena sekwestracyjnych parametrów struktur geologicznych (Effective Assessment for Sequestration Parameters of Geological Structures)* – the work of the Oil and Gas Institute – National Research Institute, and was commissioned by the Ministry of Science and Higher Education; order number: 0097/ KZ/2020, archive number: DK-4100-0085/2020.

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