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Numerical Simulations of Carbon Dioxide Storage in Selected Geological Structures in North-Western Poland

Tomasz Urych[1], *Jarosław Chećko*[1], *Małgorzata Magdziarczyk*[2] *and Adam Smoliński*[1]*

[1]*Central Mining Institute, Katowice, Poland,* [2]*Faculty of Economics and Management, Opole University of Technology, Opole, Poland*

In this study, dynamic simulation models of CO_2 injection into saline aquifers of the Choszczno-Suliszewo structure located in north-western Poland were constructed for two scenarios with different injection rates. The injection rates of 1 Mt CO_2/year and 2 Mt CO_2/year were analysed for each of the injection wells. Changes in pressures, characteristic for the sequestration process, were analysed; in addition, the spatial distribution of free CO_2 saturation in the structure and carbon dioxide dissolved in brine were presented in a graphical form. The observation time of changes occurring in the rock mass in the interval of up to 1,000 years after the completion of injection was assumed. During the modelling of CO_2 sequestration in Lower Jurassic aquifers in the Suliszewo model, the previously assumed CO_2 injection rates were achieved for both injection scenarios. The observed pressure increase does not pose any threat to the Suliszewo structure tightness. The sequestration process was found to be highly effective due to the phenomenon of the dissolution of CO_2 in brine and the resulting convection motion of brine enriched with carbon dioxide. Consequently, there is an increase in CO_2 storage capacity and permanent long-term trapping of the injected carbon dioxide. The process of the displacement of injected CO_2 from the collector layers to the layers constituting the reservoir sealing was observed. This phenomenon takes place in the upper parts of the Choszczno structure and is caused mainly by the locally occurring worse technical parameters of seal layers in this area.

Keywords: CCS—carbon capture and sequestration, simulation—computers, geological storage, greenhouse gas emission, CO_2 capture and sequestration

Edited by:
Andreas Busch,
Heriot-Watt University,
United Kingdom

Reviewed by:
Aliakbar Hassanpouryouzband,
University of Edinburgh,
United Kingdom
Chuanxiao Cheng,
Zhengzhou University of Light
Industry, China

Correspondence:
Adam Smoliński
smolin@gig.katowice.pl

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1 INTRODUCTION

In recent years, we have been observing numerous international efforts to tackle the climate crisis constituting one of the greatest challenges of our times. The number of countries committed to achieve net zero emissions by mid-century or shortly thereafter continues to grow. However, the gap between rhetoric and action needs to close if we are to stand a chance of achieving net zero by 2050 and limiting the rise in global temperatures to 1.5°C. This challenge requires a total transformation of the energy systems that underpin the economies. We are now at the beginning of a critical decade for these efforts. The 26th Conference of the Parties (COP26) of the United Nations Framework Convention on Climate Change in November 2021 was the focal point for strengthening global ambitions and actions on climate by building on the foundations of the 2015 Paris Agreement (International Energy Agency (IEA), 2021).

The main objectives of the summit were to adopt the missing implementing legislation to the Paris Agreement and to make commitments that maintain the possibility of limiting the temperature rise to 1.5°C above the pre-industrial average temperature. In light of the above, the outcome of COP26 should be considered a success—provisions on transparency, international cooperation mechanisms and a common time frame have been agreed. The final declaration adopted indicates the need to take measures to reduce global emissions by 45% by 2030 compared to 2010, and to approach climate neutrality in the middle of the 21st century. The instruments for the implementation of these activities will be, among others, the rapid building of clean generation capacities in the energy sector, accelerating the abandonment of the use of coal without CO_2 capture for this purpose, accelerated withdrawal of ineffective subsidies for fossil fuels, reduction of emissions of other greenhouse gases, but also better inclusion of the results of scientific research in the process of policy making. It was also emphasized that the transition to climate neutrality must be fair and that the protection of nature and ecosystems as natural sinks of carbon dioxide will play an important role. It was emphasized in the discussions that one cannot wait with actions to protect the climate, and the mere adoption of ambitious declarations will not stop climate change.

Despite the current gap between rhetoric and reality on emissions, there are still pathways which can help to reach net zero by 2050. It is now widely agreed that any effective response for avoiding the effects of climate change will require multiple large-scale solutions, including but not limited to new low-carbon energy production and storage (Hassanpouryouzband et al., 2021).

Moreover, carbon dioxide capture, utilisation and storage (CCUS) belongs to the technologies that can play an important role in achieving global energy and climate goals (IEAGHG, 2017; Smoliński et al., 2021; Tokarski et al., 2021). CCUS involves CO_2 capture from large emission sources, including power plants or industrial facilities that use fossil fuels or biomass as fuel; CO_2 can also be captured directly from the atmosphere. When not in use on site, the captured CO_2 is compressed and transported by pipeline, waterway, rail or road for use in a variety of applications or injected into deep geological formations (e.g., depleted oil and gas deposits or saline aquifers) for permanent and safe storage.

There are currently twenty two CCUS facilities in operation worldwide, capable of capturing more than 40 Mt of CO_2 per year (International Energy Agency (IEA), 2021). Some of these facilities have been in operation since the 1970s and 1980s, when natural gas processing plants in the Val Verde region of Texas began supplying CO_2 to local oil producers to support crude oil extraction. Since these early projects became operational, CCUS technology has been significantly developed, the range of applications has been extended and industrial scale deployment of the technology has begun. The first large-scale CO_2 capture and injection project with CO_2 storage and monitoring was commissioned at the Sleipner offshore gas plant in Norway in 1996. About 1 Mt of CO_2 per year is injected within the framework of the project and a total of more than 20 Mt of CO_2 is stored in deep saline aquifers located about 1 km below the bottom of the North Sea (Solomon, 2007). The next example of a carbon dioxide capture and storage facility is the Boundary Dam project in Saskatchewan, Canada, which was the first project to capture and store CO_2 from a coal-fired power plant on a commercial scale. The power plant was successfully modernised in 2014 and currently the capturing facility is operating at a capacity of approximately 1 Mt CO_2/year. Most of the captured CO_2 is transported via a 66 km pipeline and injected into the Weyburn oil field (EOR), while unused CO_2 is injected into a saline aquifer 2 km away as part of the Aquistore project (International Energy Agency (IEA), 2021). Another example of CCS installation is the Petra Nova project in Texas (United States), which is the world's largest post-combustion CO_2 capture system from a coal-fired power plant currently in operation. The 240 MW unit at the W.A. Parish near Houston, Texas, was equipped with a post-combustion CO_2 capture facility with a capacity of 1.4 Mt CO_2/year. The captured CO_2 was transported *via* a 130 km pipeline to the West Ranch oil field (Jackson County) for the needs of EOR. Currently, the Petra Nova installation in the United States has temporarily suspended CO_2 capture operations due to low oil prices (International Energy Agency (IEA), 2021).

Stronger investment incentives and set climate targets are generating a new momentum for CCUS technology. Plans to build more than 30 commercial CCUS facilities have been announced in recent years. Many of these plans involve the development of industrial hubs that combine CO_2 capture from a range of facilities with shared infrastructure for CO_2 transport and storage. The examples include the Alberta Carbon Trunk Line (ACTL) project in Canada[1], which became operational in 2020, and the planned Longship project in Norway[2]. CO_2 storage involves injecting captured carbon dioxide into deep geological formations of porous rocks covered by an impermeable rock layer which seals the reservoir and prevents it from migrating towards the land surface or "leaking" into the atmosphere. There are several types of reservoirs suitable for CO_2 storage, inter alia deep saline aquifers and depleted oil and gas fields, which have the highest storage potential. Deep saline aquifers are layers of porous and permeable rocks saturated with brine which are widespread in both onshore and offshore sedimentary basins. In contrast, depleted oil and gas reservoirs are porous rock formations that have held oil or gas for millions of years prior to extraction and may similarly allow permanent storage of injected CO_2. When carbon dioxide is injected into a geological structure, it moves to fill the pore spaces in the rocks. The gas is usually compressed first to increase its density, and the potential reservoir typically needs to be at depths greater than 800 m to ensure that the injected CO_2 remains in a supercritical state.

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[1] https://actl.ca.

[2] https://ccsnorway.com/report-developing-longship-key-lessons-learned.

Carbon dioxide is permanently trapped in the reservoir by the following mechanisms (Juanes et al., 2006): structural trapping in which low-permeability overburden rocks provide a seal to the reservoir (Rosenbauer and Thomas, 2010; Zhang and Song, 2014); dissolved trapping in which CO_2 dissolves in the brine that fills the rock pores (Leonenko and Keith, 2008; Han et al., 2011); residual trapping where CO_2 becomes trapped in pore spaces in the rocks due to capillary forces (Pini et al., 2012; Li et al., 2017); mineral trapping whereby CO_2 can react with minerals and organic matter in the geological formation, as a result of which carbonate minerals are formed through mineralisation and carbon dioxide becomes permanently bound to the rock matrix (Rochelle et al., 2004; Farajzadeh et al., 2009).

The nature and type of trapping mechanisms to provide permanent and effective CO_2 storage, which vary depending on the geological conditions within a reservoir (Rosenbauer et al., 2005), are well understood owing to years of experience gained from projects involving CO_2 injection through Enhanced Oil Recovery—EOR (Le Gallo et al., 2002; Godec et al., 2011), Enhanced Gas recovery—EGR (Van der Meer, 2005; Raza et al., 2018), Enhanced Coalbed Methane recovery - ECBM (Shi et al., 2005; Vishal, 2017), and CO_2 storage in deep saline aquifers (Balashov et al., 2013; Bachu et al., 2014).

Moreover, there have been other applications for geological CO_2 storage such as hydrocarbon recovery from unconventional hydrocarbon reserves (e.g., gas hydrates). CO_2 sequestration and storage into methane (CH_4) hydrate sediments are investigated (Jadhawar et al., 2021) to evaluate CH_4 replacement by CO_2 in hydrates through both the macroscale and microscale experiments under varying thermodynamic conditions. Various approaches of CO_2 sequestration via gas hydrates are possible, including storage in seawater, sediments under the sea floor, permafrost regions, and methane hydrate reservoirs via CO_2-CH_4 exchange and depleted gas fields (Zheng et al., 2020).

CO_2 storage in magmatic rocks (basalts), which have high concentrations of reactive chemicals, is also possible but is still at an early stage of development. Under this technology, the injected CO_2 reacts with chemical components to form stable minerals in the rocks and, simultaneously, traps carbon dioxide in geological formations (Goldberg et al., 2008; Matter et al., 2011; Gysi and Stefánsson, 2012). Global resources for CO_2 storage are believed to far exceed likely future demand. The International Energy Agency scenarios assume that CCUS technologies will play an important role in reducing CO_2 emissions in the industrial and energy sectors.

In the IEA Sustainability Scenario (International Energy Agency (IEA), 2020), in which global CO_2 emissions from the power sector fall to zero on a net basis by 2070, CCUS technology accounts for almost 15% of the cumulative emissions reductions compared to the Stated Policies Scenario (STEPS). The contribution of CCUS is steadily increasing and covers almost all parts of the global energy system. However, significant further research work is needed in many regions to convert theoretical storage capacity into estimates of 'bankable storage' status to support CCUS investments (Heddle et al., 2003; Balat and Öz, 2007; Smoliński et al., 2021). The availability and recognition of suitable geological formations and structures for underground CO_2 storage still remain the key factors which limit the possibility of using CCS technology in climate plans. The selection of a suitable underground geological formation for permanent CO_2 storage must be preceded by a detailed characterisation and assessment of the potential storage reservoir and the surrounding rock mass (Buscheck et al., 2012; Tokarski et al., 2021). The characterisation of the dynamic behaviour of carbon dioxide stored in the rock mass is an important step in the process of evaluating a potential CO_2 reservoir (Kumar et al., 2020). Numerical modelling includes a series of simulations of the CO_2 injection process into the storage site using a 3D static geological model of the rock mass. Available software packages for simulating phenomena related to the geological carbon dioxide storage process are mainly developed based on source codes of reservoir simulators used in the oil and gas industry. Jiang (Jiang, 2011) conducted a comparison of available reservoir simulators used for the numerical analysis of geological storage of carbon dioxide. The analysis shows that numerical simulations depend on the simulator used, characterised by the physical models used, numerical methods and specific discretisation methods. The results of numerical simulations determine the estimated CO_2 storage capacities in geological structures, which are a key element in the decision-making process when considering the implementation of CCS projects on an industrial scale.

Within the framework of modelling dynamic behaviour of CO_2 storage in the subsurface, researchers have proposed various numerical models. There are many case studies of CO_2 storage around the world such as Johansen formation (Eigestad et al., 2009), Utsira formation (Møll Nilsen et al., 2015), Cranfield pilot project (Delshad et al., 2013), pilot project in Frio brine formation (Ghomian et al., 2008) to list but a few. Some review articles summarized the different physico-chemical methods responsible for suitable CO_2 storage and the difficulties in other aspects (Riaz and Cinar, 2014; Aminu et al., 2017; Belhaj and Bera, 2017; Thakur et al., 2018). Moreover, Ajayi et al. (Ajayi et al., 2019) present all aspects of CCUS projects worldwide along with the technologies, modelling issues and physico-chemical processes occurring during the CO_2 storage within geological formations.

Research activities into CCS in Poland encompass both theoretical works on the modelling of CO_2 injection processes into geological formations (Tarkowski and Uliasz-Misiak, 2002; Scholtz et al., 2006; Tarkowski, 2008; Vangkilde-Pedersen et al., 2009) and experiments of small-scale CO_2 injection into the Borzęcin gas deposit (Lubaś, 2007) and the Kaniów coal deposit (Van Bergen et al., 2009). In addition, intensive activities were carried out in Poland regarding the possibility of storing CO_2 in saline aquifers (Uliasz-Misiak, 2007; Nagy and Siemek, 2009; Stopa et al., 2009; Solik-Heliasz, 2011). A number of formations and structures located in the area of Poland were analysed during the conducted research (Bromek et al., 2009; Jureczka et al., 2012; Wójcicki, 2012; Urych and Lutyński, 2019; Chećko et al., 2020; Koteras et al., 2020) in terms of safe CO_2 storage and the potential for CO_2 storage in saline aquifers in the Upper Silesian Coal Basin using numerical modelling methods (Urych and Smoliński, 2019). Additionally, potential geological structures for CO_2 storage in formations occurring in the Polish

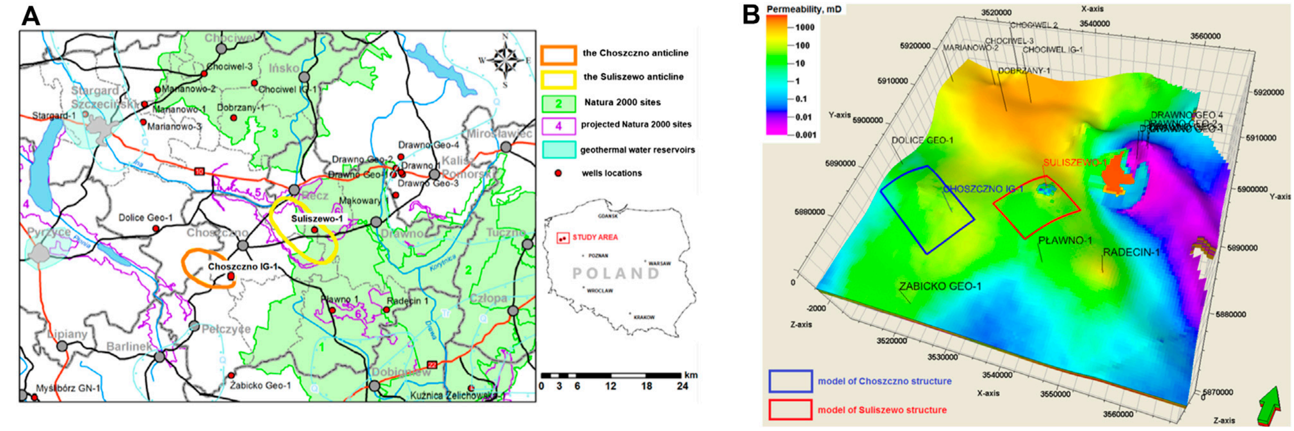

FIGURE 1 | Choszczno-Suliszewo area: **(A)** Location map and **(B)** structures delineated in a static numerical model.

Lowlands were characterized in detail (Marek et al., 2010), including the possibility of using the anticlines of Choszczno and Suliszewo for underground CO_2 storage (Dziewińska and Tarkowski, 2012; Marek et al., 2013).

The objective of this paper is to present the results of numerical simulations of the CO_2 storage process in brine aquifers in the area of Choszczno and Suliszewo anticlines located in the Szczecin Trough in north-western Poland. Model tests and numerical simulations were carried out using the Petrel Reservoir Engineering software (Schlumberger Information Solutions, 2010) cooperating with the ECLIPSE reservoir simulator (Schlumberger Information Solutions, 2011).

2 MATERIALS AND METHODS

2.1 Location of the Study Area, Land Use and Geological Structure

Two anticlinal structures, Choszczno and Suliszewo, Poland, were selected for the simulation of CO_2 injection into brine aquifers. Both are located in the north-western part of Poland. The Choszczno structure is situated in the vicinity of the towns of Pełczyce and Choszczno (**Figure 1**). The area of the studied reservoir is characterised by a dispersed rural development with some forested areas. Arable fields and meadows play a dominant role. The studied area is situated within a distance of 25 km from Pyrzyce and Stargard Szczeciński which use or previously used the heat obtained from geothermal waters. The Suliszewo anticline is located approximately 12 km from the Choszczno reservoir (**Figure 1**). Similarly to the Choszczno structure, this area is also dominated by meadows and arable fields with a slightly higher share of woodlands. Within the boundaries of the Suliszewo reservoir there are both already functioning and planned protected areas established within the Natura 2000 programme. The analysed areas were identified on the basis of the well data and seismic surveys. One deep well was drilled in the area of potential reservoirs and the remaining ones are situated at considerable distances from the analysed areas. A relatively high density of wells is observed north-east of the Suliszewo Reservoir in the area of Kalisz Pomorski (**Figure 1**), with the remaining wells distributed in irregular grid pattern mainly north and south of the studied areas. The seismic survey profiles, mostly running NE-SW and NW-SE, provide valuable information for studies.

The overburden of the potential reservoirs in the studied area consists of Quaternary, Tertiary, Cretaceous and Upper and Middle Jurassic sediments. The Quaternary sediments consist of clays, gravels, sands and silts which were formed as a result of glacial and interglacial processes. The thickness of the Quaternary cover in the Choszczno reservoir area is 148 m, and in the case of Suliszewo—163 m. The Tertiary sediments in the studied area are characterized by variable thickness from about 3 m in the Choszczno area to 63 m in the Suliszewo area. The Tertiary sediments are Middle Miocene sediments consisting mainly of dark brown clays with inclusions of silts and very fine-grained clay sands. The lithology of the Upper Cretaceous is dominated by marls, marly and pelitic limestones as well as marly opaques. The thickness of the Upper Cretaceous in the studied area is approx. 800 m. The Lower Cretaceous sediments (Albian, Hoterivian) in the upper part of the profile are formed by marly limestones, while in the lower part by marly-sandy and clay-sandy formations. The Lower Cretaceous sediments in the south-western part of the Szczecin Trough are considerably reduced—their thickness ranges from 5 to 30 m. The thickness of the Lower Cretaceous sediments in the studied area ranges from 12.5 m (the Choszczno reservoir) to 20 m (the Suliszewo reservoir). In the formations of the Upper Jurassic, Lower and Middle Oxfordian sediments are distinguished. The Lower Oxford is represented by marl and marly siltstone sediments, whereas the Middle Oxford is represented by siltstone with insets of mudstone, oolitic limestone and marly siltstone. The Middle Jurassic sediments are characterised by bipartite character. The upper part of the profile is formed by Upper Jurassic sediments composed of sandy and marly mudstones, underlain by marly dolomites and dolomitic mudstones. The total thickness of the Upper and Middle Jurassic sediments in the studied area ranges from 167 to 180 m. The Lower Jurassic Gryfice Beds (Lower

TABLE 1 | Details of the reservoir simulation model and parameters of reservoir horizon of the Lower Jurassic Komorowo Beds (Michna and Papiernik, 2012; Luboń, 2021).

Model parameter	Suliszewo model	Choszczno model
Model area, km^2	210	330
Grid dimension, m	3,000 × 2,625	3,300 × 3,050
3D mesh resolution, m	56 × 48 × 24	83 × 48 × 24
Average porosity, %	26.2–27.6	24.6–26.1
Average permeability, mD	2,719.5–3,582.4	2,209.9–2,831.6
Clay mineral content, %	10–19	14–23

Toarcian) of thickness ranging from 40 m (Suliszewo) to 70 m (Choszczno), which are divided into two sections, the upper and the lower, constitute the formations sealing the reservoir series. The upper section is comprised mainly of siltstones and mudstones, whereas the lower section is represented by marine ingression sediments containing mainly clay shales with inserts of siderite and dolomitic sandstone.

The most favourable parameters for carbon dioxide storage within the Choszczno and Suliszewo structures are found in the Lower Jurassic Komorowo Beds of the Upper Pliensbachian (Domerian) age and the Radów and Mechów Beds of the Synemurian. They are built mainly of fine-grained sandstones with clay inserts. The thickness of the Komorowo Beds in the Szczecin Trough ranges from 70 to 180 m; for the Choszczno Reservoir, it is 100 m, and for Suliszewo—about 80 m. The thickness of the Radów and Mechów Beds is 120 and 80 m, respectively. The sediments of the Łobez Beds constitute a series that underlies the Komorowski strata. The age of the Łobez Beds was determined as Lower Pliensbachian—Carix. In general, the Łobez Beds in the Szczecin Trough are composed of silt, clay and sandy sediments. The thickness of the series underlying the Komorowo Beds in the area of the analysed reservoirs ranges from 20 m (Choszczno) to 40 m (Suliszewo). Below the reservoir formations, there occur dark grey claystones of the Upper Triassic (the Rhaetian) (Dadlez, 1979).

2.2 Description of Simulation Model

A structural and parametric model developed for the Lower Jurassic reservoir formation located in the Radęcin-Suliszewo area (Michna and Papiernik, 2012) was used for numerical simulations of the process of CO_2 injection into saline aquifers. The initial model was constructed on the basis of a regular grid of 116 × 120 cells with surface dimensions of 500 × 500 m. In this model, two regions were separated (**Figure 1**) in which simulations of CO_2 injection into saline aquifers were carried out. The effective porosity of the simulation models of a potential CO_2 deposit ranges from 26.2 to 27.6% for the Suliszewo structure and from 24.6 to 26.1% for the Choszczno structure. The permeability of the Suliszewo model ranges from 2,719.5 to 3,582.4 mD, whereas that of the Choszczno model—from 2,209.9 to 2,831.6 mD. The content of clay minerals ranges from 10 to 19% for the Suliszewo structure and from 14 to 23% for the Choszczno structure. Detailed characteristics of numerical models are summarized in **Table 1**.

2.2.1 Description of Suliszewo Model

In the first of the separated numerical models, covering an area of about 210 km^2, situated in the area of the Suliszewo-1 well, the

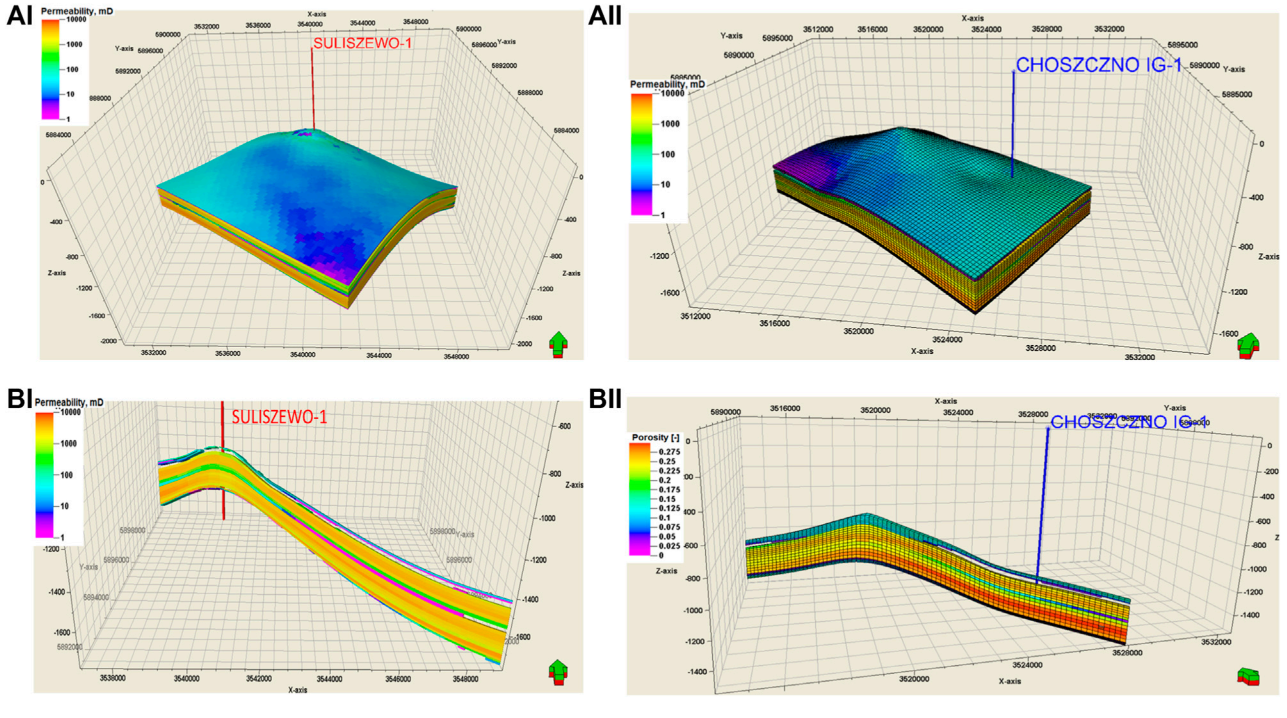

FIGURE 2 | Numerical model in the **(I)** Suliszewo-1 and **(II)** Choszczno IG-1 well area: **(A)** Permeability model, **(B)** hydrodynamic discontinuity in the porosity model.

TABLE 2 | CO_2 solubility (R_{sb}) and CO_2 formation volume factor (B_w) as function of pressure (P_w) (Chang et al., 1996).

R_{sb} (sm^3 CO_2/sm^3 brine)	P_w (bar)	B_w (rm^3/sm^3)
0.56850	1.0132	1.01765
19.2812	54.288	1.04267
26.5999	107.564	1.04267
29.8362	160.840	1.05232
32.6200	267.391	1.05878
33.5212	320.667	1.06021
34.3937	373.943	1.06139

horizontal grid resolution (200 × 200 m) and the orientation of the grid lines in NW-SE and perpendicular directions were modified (**Figure 2**). This resulted in a model with a cell resolution of 56 × 48 × 24 (64,512 cells). A *cut-off* method was then applied for permeability (0.01 mD), porosity (0.5%) and clay mineral content (70%). Hydrodynamic discontinuities were found in the Toarcian layers forming the seal of the Pliensbachian collector (**Figure 2**).

2.2.2 Description of Choszczno Model

The simulation model, located in the Choszczno IG-1 well site area, covers about 330 km^2. The horizontal grid resolution in this model is 200 × 200 m and grid lines are oriented in NW-SE and perpendicular direction (**Figure 2**). Originally, the Choszczno model consisted of 95,616 cells (83 × 48 × 24), but after excluding from the simulation cells with permeability <0.01 mD, porosity <0.5%, and clay mineral content >70%, the final number of active cells is 78,910. The sealing layers in the Choszczno model are characterized by worse properties in comparison with analogous overburden rocks of the Suliszewo model analysed earlier. The modelled sealing of the reservoir in this region has lower values of clay mineral content (42–60%) than in the remaining part of the model (over 70%), especially in some areas of the upper part of the structure. The permeability of seal layers in the upper part of the structure ranges from 12 to 61 mD, and porosity—from 10 to 16%. After the application of the *cut-off* method for permeability and clay mineral content, a hydrodynamic discontinuity was found in the Toarcian layers forming the seal of the Pliensbachian collector. The *cut-off* parameter values used had the effect of deactivating the poorly permeable part of the Pliensbachian layers, but leaving a connection to the overlying layers at the top of the structure (near the injection well). Therefore, the part of the Choszczno model cells located at the top of the structure could not be considered as sufficient sealing of the reservoir and numerical simulations of the tightness of the structure had to be developed (**Figure 2**).

2.3 Models of Reservoir Fluids and Boundary Conditions

A composite version of the ECLIPSE simulator (E300) was used to simulate the process of the injection of carbon dioxide into saline aquifers in the Choszczno-Suliszewo region. In the dynamic models, the CO2SOL option was applied which takes into account the phenomenon of carbon dioxide solubility in the aqueous phase in the sequestration process. The Peng-Robinson equation of state was used with a slight modification concerning the molar volume, thanks to which the thermodynamic parameters of carbon dioxide are determined in a manner more similar to real conditions (Eclipse User Manual, 2011). The ECLIPSE reservoir simulator defines the sm^3 unit as a cubic meter of gas at pressure 1,013.25 hPa and temperature equal to 15.56°C. The unit rm^3 describes the volume of gas at reservoir conditions (Eclipse User Manual, 2011). Carbon dioxide viscosity was estimated using the Lorentz-Bray-Clark correlation (Lorentz et al., 1964). Parameters for CO_2 solubility in brine were determined from the Chang-Coats-Nolen correlation (Chang et al., 1996). Aqueous phase properties follow the correlations used in the numerical model are presented in **Table 2**.

The flow of carbon dioxide in layers saturated with water (brine) is controlled by the curves of relative permeability. Due to the fact that the authors did not have the results of the tests on the borehole cores, in this study the general liquid permeability and capillary pressure characteristics of van Genuchten (Van Genuchten, 1980) were used; relative gas permeability curves

TABLE 3 | Characteristics of reservoir properties and initial conditions of the simulation models.

	Parameter	Value
Properties of reservoir water	Density d_w, kg/m^3	1,009.3
	Viscosity $\mu_{w,}$ cP	0.9957
	Compressibility $c_{w,}$ 1/Pa	3.215×10^{-10}
	Volumetric coefficient B_w, rm^3/sm^3	1.0330
Initial conditions	Average temperature, °C	38.0
	Initial reservoir pressure, MPa	10.74
	Reference depth, m	1,069
Cut-off parameters	Permeability, mD	<0.01
	Porosity, %	<0.50
	Clay mineral content, %	>70
Carter-Tracy analytical aquifer parameters	External radius, m	500
	Thickness, m	50
	Angle of influence, deg	360
	Total (rock + water) compressibility, 1/bar	0.00001

TABLE 4 | Summary of injection rates for different simulation variants.

Model name	Surface ordinate, m asl	Injection ordinate CO_2, m asl	Simulation scenario	Injection capacity, sm^3/d	Total quantity CO_2, Mt
Suliszewo	95.0	from −1,187.0 to −1,207.0 (Pliensbachian) and from −1,285.5 to 1,306.0 (Sinemurian)	1 2	1,449 667 2,899 334	25 50
Choszczno	98.5	from −1,123.5 to 1,140.5 (Pliensbachian) and from −1,244.5 to 1,267.0 (Sinemurian)	1 2	1,449 667 2,899 334	25 50

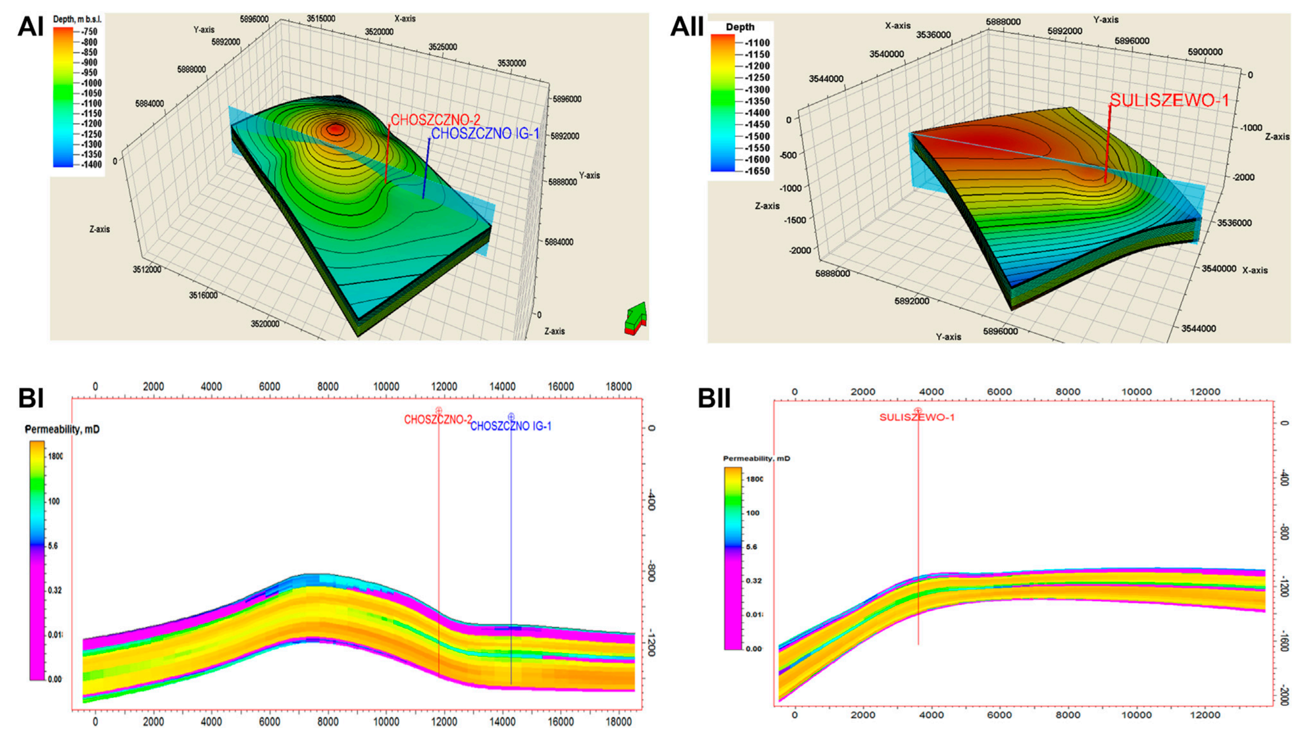

FIGURE 3 | (A) Location of the injection well in the **(I)** Choszczno and **(II)** Suliszewo structure; **(B)** cross-section through the structure in the area of the Choszczno-2 and Suliszewo injection wells, respectively.

were generated based on Corey's correlation (Corey, 1954; Doughty and Pruess, 2004).

In the initial phase of the simulation, the model is 100% saturated with brine with salinity of 12.9 g/dm^3 and density of 1,009.3 kg/m^3. The gas-water contact depth position, which was defined above the minimum model depth, was taken as the initial condition for the reservoir simulations carried out. The initial reservoir pressure at the depth of 1,069 m, amounting to 107.4 bar, was determined from measurements in the Radęcin-1 well. The average temperature of 38°C at the depth of 1,000 m was assumed. Fluids at the above mentioned pressure and reservoir temperature were in hydrostatic equilibrium conditions.

The numerical model was defined as open due to the lack of surface constraint of the analysed structure in the Lower Jurassic; in addition, the influence of the hydrodynamic openness of the geological structure on the CO_2 storage process was considered. The aquifers surrounding the area covered by the numerical model were simulated using semi-analytic models of aquifers defined by Carter and Tracy (Carter and Tracy, 1960) developed for calculating water influx behaviour. The initial pressure in the analytical aquifer is similar to that in the numerical model, and the other parameters of the aquifer were taken as average quantities from the area of the numerical model. The simulation model was initiated at an average reservoir pressure of 10.74 MPa and temperature of 38°C at the depth of 1,069 m with a gradient of 0.03°C/m. The basic initial parameters assumed in each simulation model are summarised in **Table 3**.

2.4 Model Study Design

The simulations of the CO_2 storage process in brine aquifers were carried out using vertical wells. For each of the two numerical models, two process simulation scenarios with

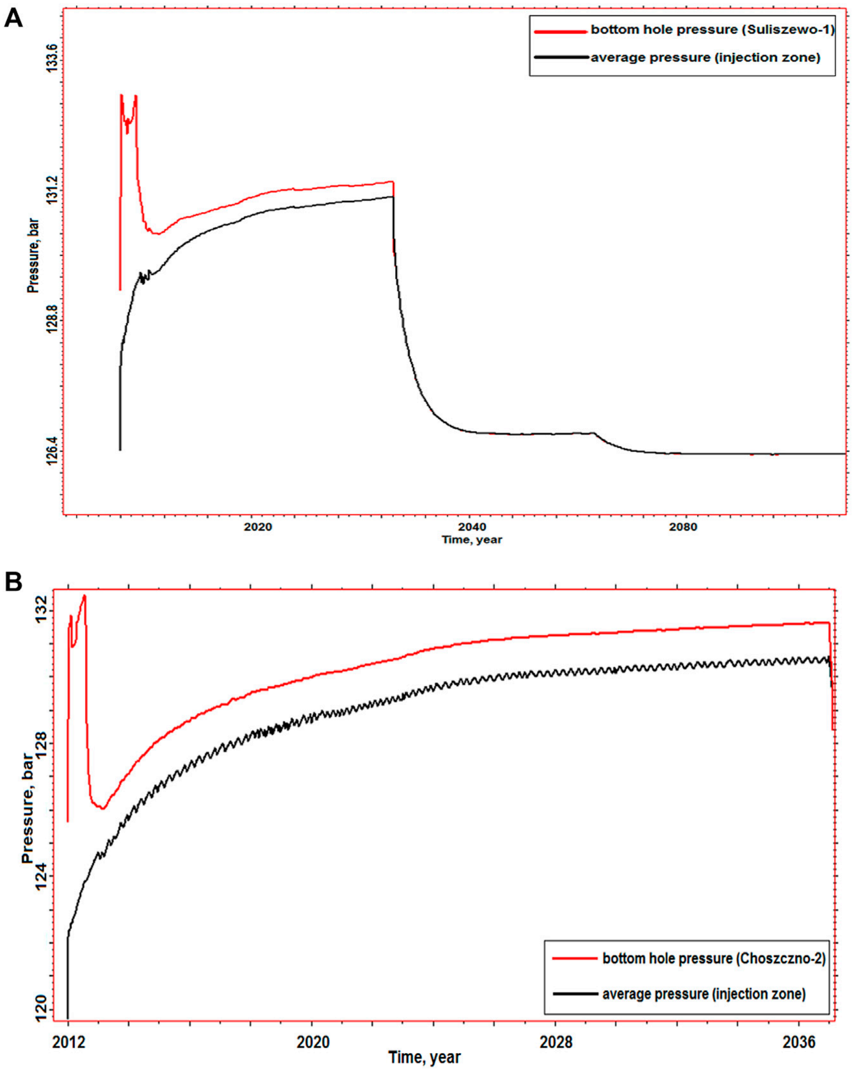

FIGURE 4 | Bottomhole pressure in the **(A)** Suliszewo-1 and **(B)** Choszczno-2 well and average formation pressure in the injection zone.

different injection rates were adopted. The numerical simulations performed under Scenario no. 1 cover the injection at a capacity of 1 Mt CO_2/year. Scenario no. 2 concerns an injection capacity of 2 Mt CO_2/year. Therefore, the total amount of injected carbon dioxide under Scenario no. 1 is 25 Mt, and under Scenario no. 2 it is 50 Mt. Constant injection rate and maximum bottom pressure in the P_{BHP} injection well were assumed as boundary conditions of the analysed process. The simulations of CO_2 migration process in the analysed structure were carried out for 200-year and 1000-year time intervals after the completion of the injection. The simulations assumed the injection of CO_2 in one well in the area of each anticline, at two depth intervals. Carbon dioxide is injected into the roof layers of the Pliensbachian and Sinemurian collectors (**Table 4**). The choice of the location of injection wells was considered in view of the efficiency of the sequestration process. In the Choszczno Reservoir, the Choszczno-2 injection well was located at a distance of about 2.5 km from the Choszczno IG-1 well (**Figure 3**), whereas in the Suliszewo Reservoir area, CO_2 injection was planned in the existing Suliszewo-1 well (**Figure 3**).

3 RESULTS AND DISCUSSION

3.1 Simulation Results for Model of Suliszewo Structure – Scenario 1

In the course of CO_2 injection simulations for Scenario no. 1, a constant daily injection rate of about 1,449 667 sm^3/d was maintained in the Suliszewo model, which corresponds to a total quantity of injected CO_2 equal to 25 Mt of CO_2. The pressure at the bottom of the injection well drops sharply after the injection is completed; and in the further stage of the simulation, it reaches the original pressure. The bottom pressure in the injection well changes by about 3.5 bar,

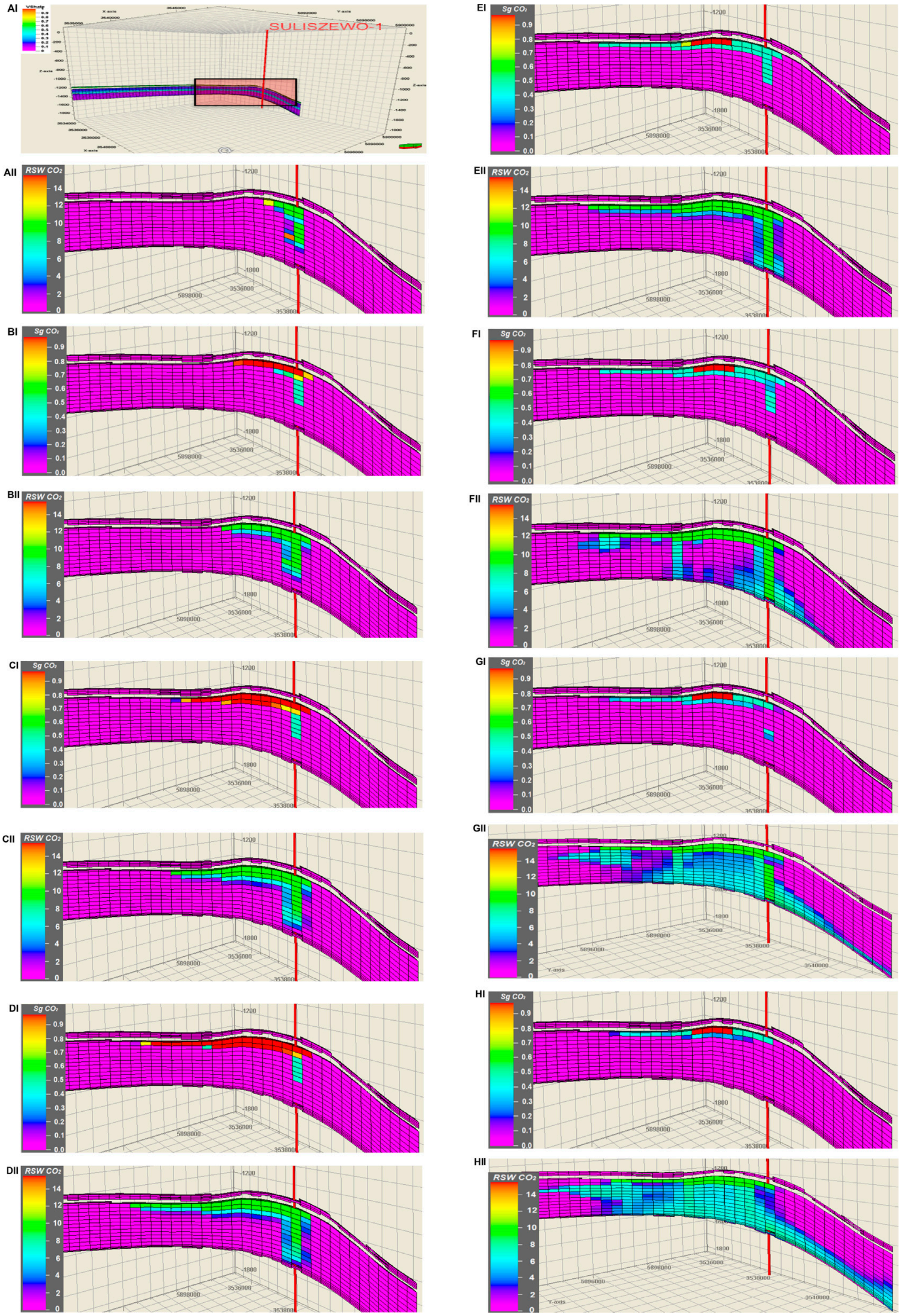

FIGURE 5 | Determined section enlarged in the **(I)** distribution of free CO_2 saturation in the structure and **(II)** structure saturation distribution of CO_2 dissolved in brine (RSW_{CO2}-molar fraction) after **(A)** 5, **(B)** 15, **(C)** 20, **(D)** 25, **(E)** 50, (f) 200, **(G)** 500 and **(H)** 1,000 years from the start of injection.

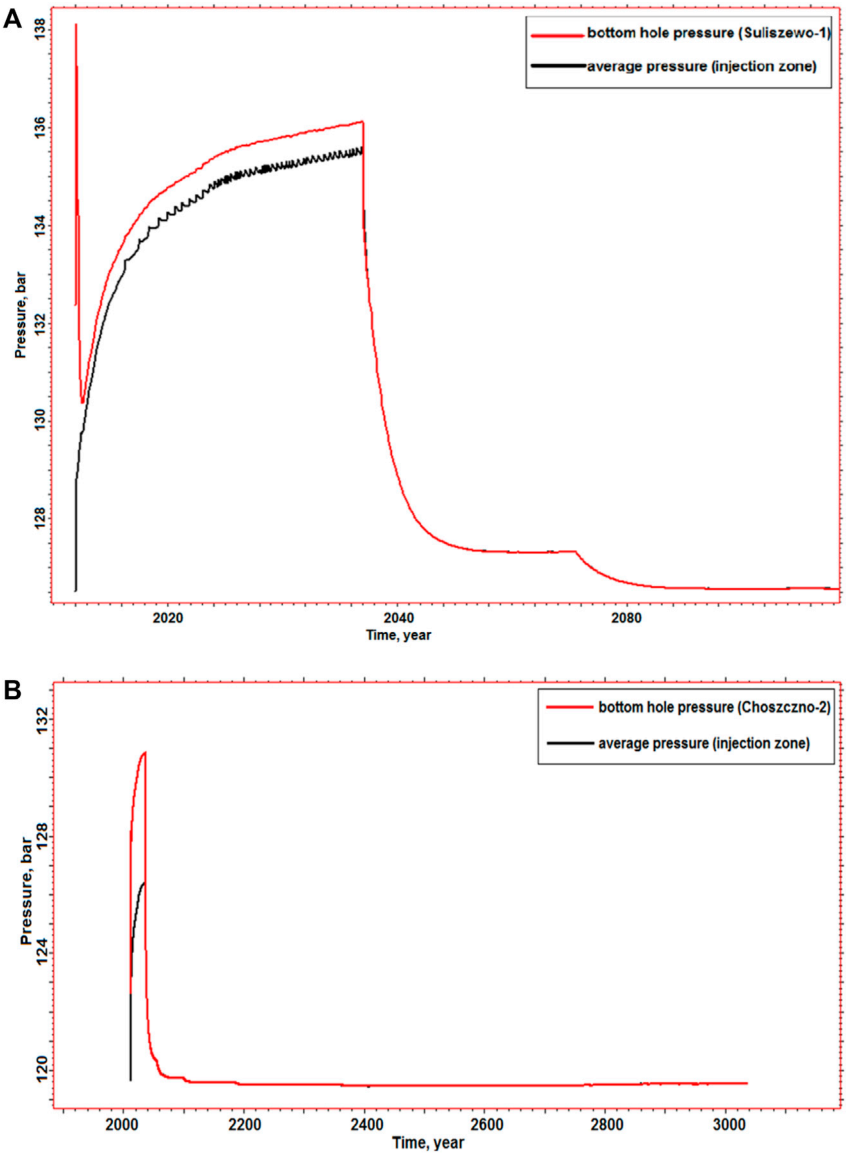

FIGURE 6 | Bottom pressure in the **(A)** Suliszewo-1 and **(B)** Choszczno-2 wells, respectively and average formation pressure in the injection zone during and after injection.

while the average pressure in the injection zone changes by about 4 bar (**Figure 4**).

The pressure increase in the collector roof layers is a maximum of about 5 bar after 25 years elapsed from the injection. In the following years, a pressure drop was observed in the upper parts of the structure due to the dissolution of CO_2 in brine and its further migration in the collector roof layers. As a result of long-term simulations carried out for a further 1,000 years after the completion of the injection, it was found that after about 70 years the pressure in the roof is close to the original pressure before the start of the injection. In the initial phase of the simulation, the injected carbon dioxide accumulates in the region of the injection hole. Due to the differences in properties of individual layers of the model, as well as due to buoyancy forces and reservoir pressure gradient, a concentration of free CO_2 is observed in the upper layers of the collector. With time, there is a slow movement of carbon dioxide along the collector roof in the S-E direction. The distribution of the saturation of the structure with the carbon dioxide remaining in the residual state for particular time intervals of the simulation is presented on cross sections passing through the near-well zone (**Figure 5**).

During the process of gravitational migration of CO_2 towards the local top of the structure, the dissolution of

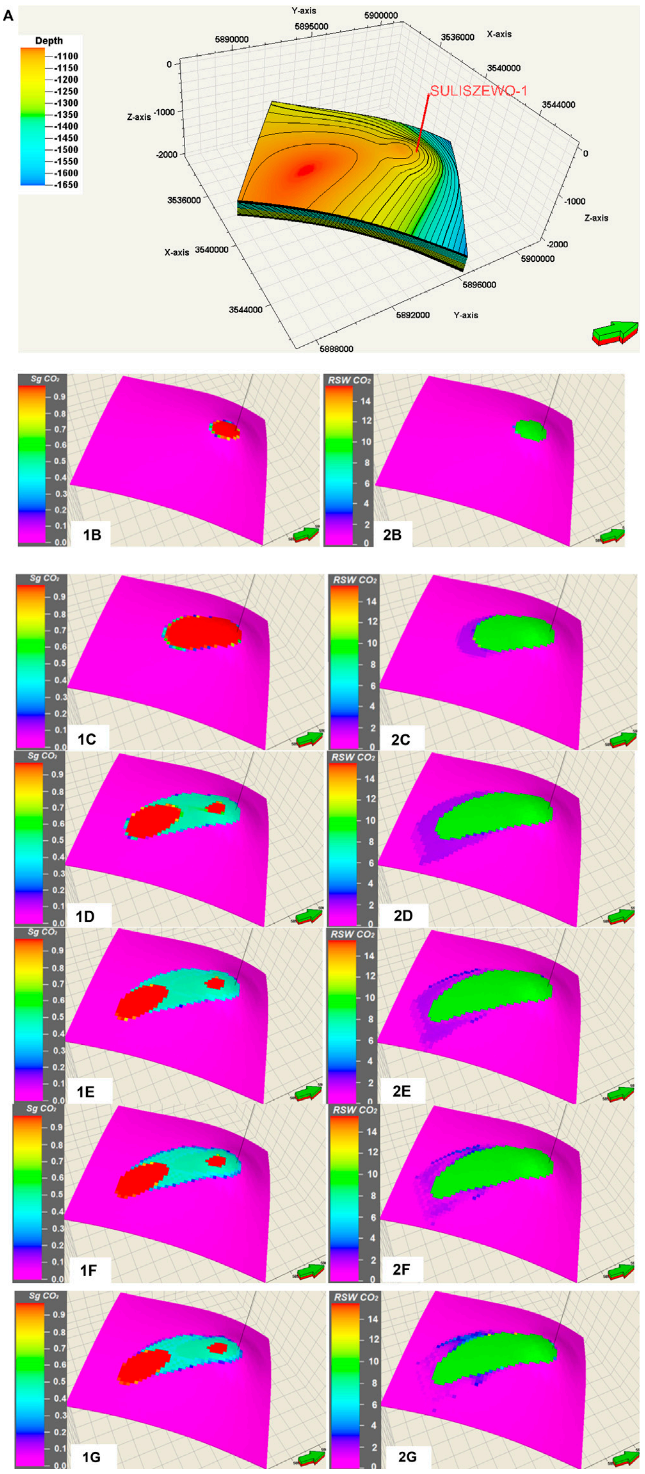

FIGURE 7 | Determined section enlarged in the following Figures **(A)**, the distribution of free CO_2 saturation **(1)** and CO_2 dissolved in brine RSWCO2-molar fraction **(2)** in the roof layer of the Pliensbachian collector after **(B)** 5, **(C)** 25 years of injection and after **(D)** 50, **(E)** 200, **(F)** 500, **(G)** 1,000 years after the completion of injection.

carbon dioxide in brine takes place. The longer the gas migration time, the greater is the possibility that the CO_2 will dissolve and remain in the pore spaces of the rocks. The distribution of dissolved CO_2 in the analysed structure is presented by molar fractions for individual simulation time intervals (**Figure 5**). In the following Figures, a slow reduction process of the free phase of CO_2 can be observed due to the fact that CO_2 dissolves in brine and falls towards the lower layers of

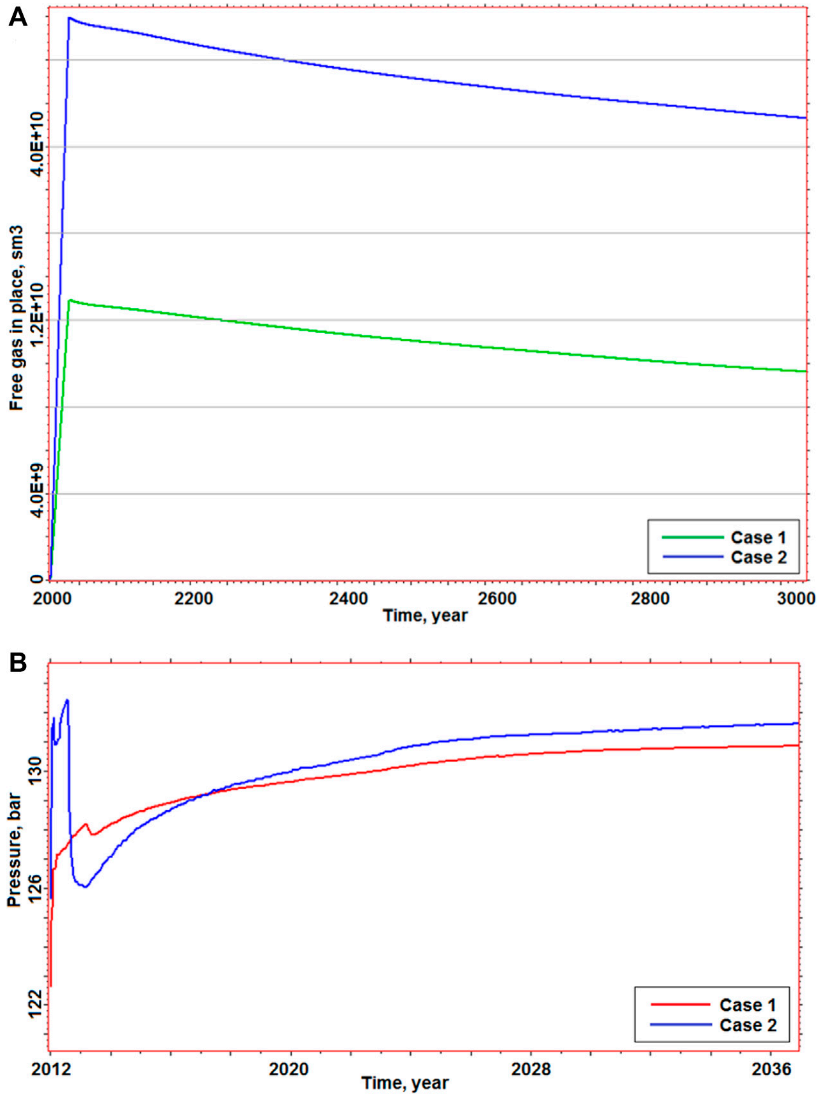

FIGURE 8 | Comparison of changes in the quantity of free CO_2 over time in the structure for Scenarios no. 1 and no. 2 in the **(A)** Suliszewo and **(B)** Choszczno-2 structures.

the collector. The brine convection phenomenon occurs due to the changes in its density caused by CO_2 dissolution.

3.2 Simulation Results for Model of Suliszewo Structure—Scenario 2

The results of CO_2 injection simulations for Scenario no. 2 in the Suliszewo model show a constant daily injection rate of about 2,899 334 sm^3/d, which corresponds to a total amount of injected CO_2 equal to 50 Mt. Similarly as in the case of Scenario no. 1, the pressure at the bottom of the injection well drops sharply after the injection is completed; in the further stage of the simulation it tends to reach the original pressure. The bottom pressure in the injection well changes by about 4 bar, while the change in average pressure in the injection zone is about 7 bar (**Figure 6**). The pressure increase in the collector roof layers is a maximum of about 9.5 bar after 25 years of the injection process. However, after the injection has been completed, the roof pressure decreases and only about 1.5 bar increase of the original roof pressure of the structure was already observed about 10 years after the injection had finished.

In this injection scenario (2 Mt CO_2/year), the formation and gradual development of free CO_2 zones around the injection well takes place. It is also noticeable that CO_2 moves towards the collector roof layers and further towards the local top of the structure due to the prevailing buoyancy forces. In addition, the phenomenon of CO_2 dissolution in brine occurs here. The Figures below

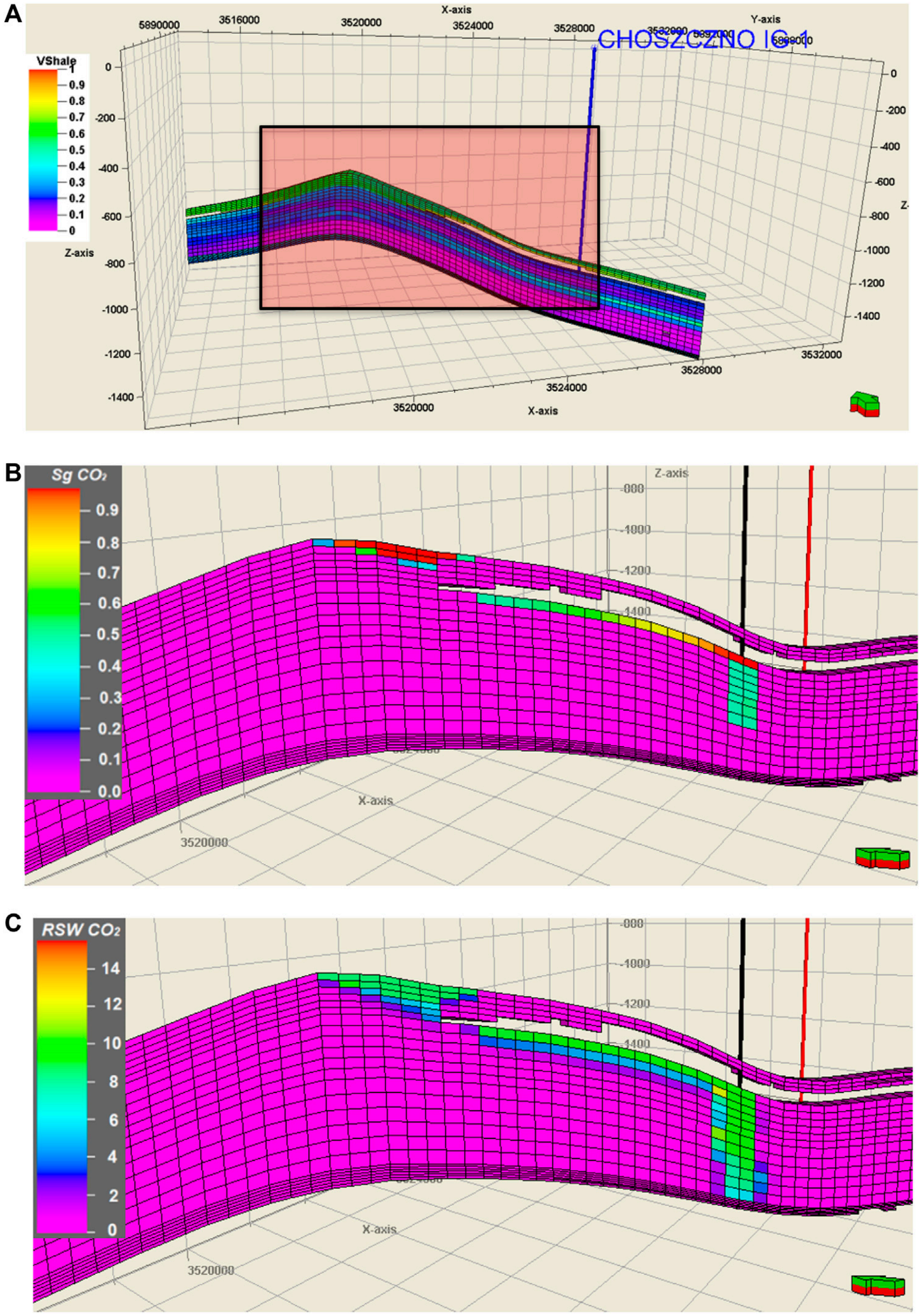

FIGURE 9 | The determined fragment of the section enlarged in the following Figures **(A)**, the distribution of free CO_2 saturation in the structure **(B)** and the distribution of CO_2 saturation dissolved in brine **(c)** after 25 years of injection.

(**Figure 7**) show the changes in saturation of free CO_2 (Figures on the right) and dissolved CO_2 (Figures on the left) for the same time intervals. It is evident that the brine containing dissolved CO_2 spreads over a much larger area compared to the residual CO_2 zone.

Figure 8 shows the dissolution rate of the injected carbon dioxide in brine for two simulation scenarios. The course of the CO_2 dissolution process in brine largely depends on the effective contact area between carbon dioxide and brine.

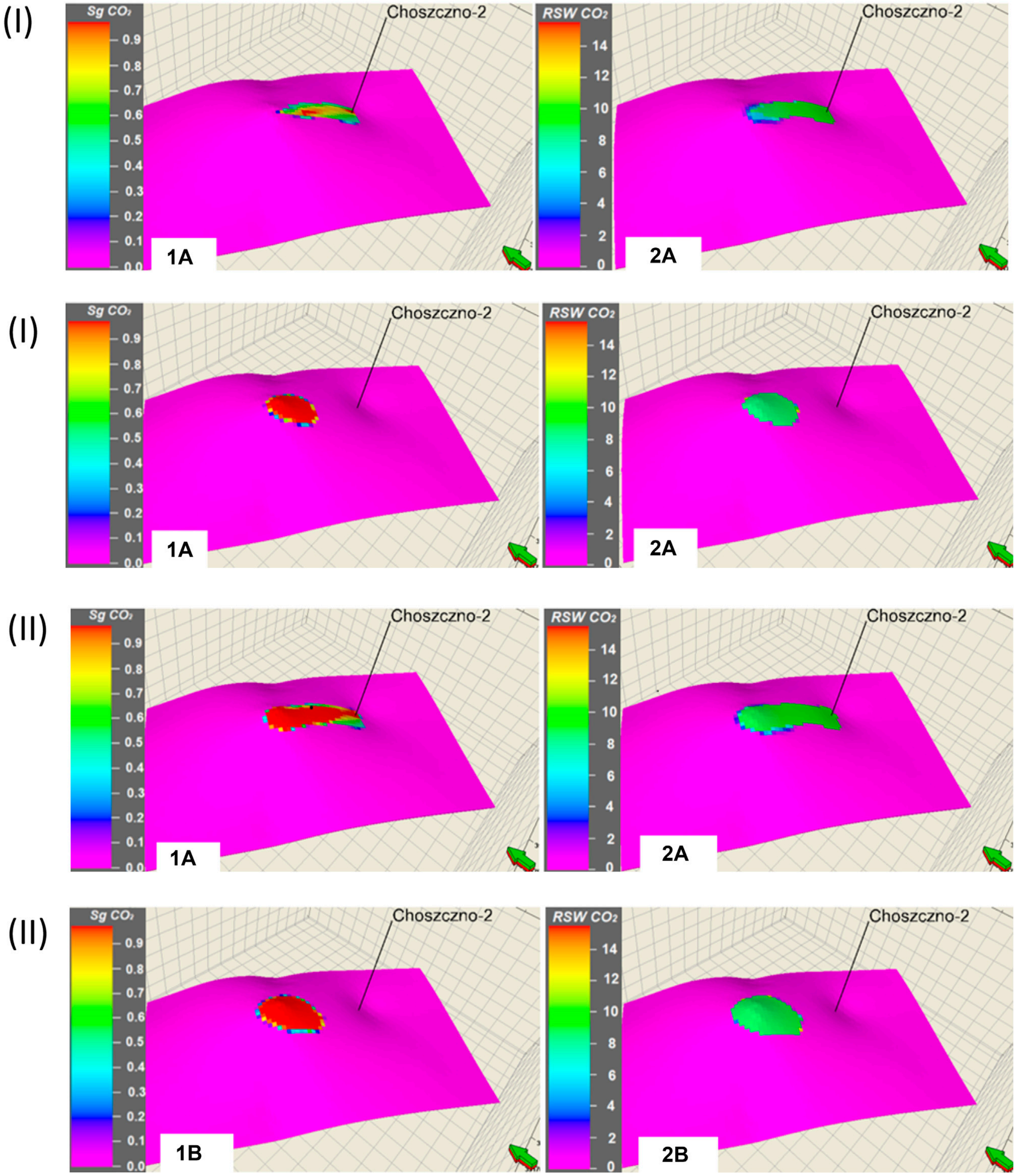

FIGURE 10 | Distribution of saturated free CO_2 **(1)** and dissolved CO_2 **(2)** in the **(I)** Pliensbachian collector roof layer and **(II) (A)** and in the sealing roof layer **(B)** in the sealing roof layer of the Toarcian after 25 years of injection.

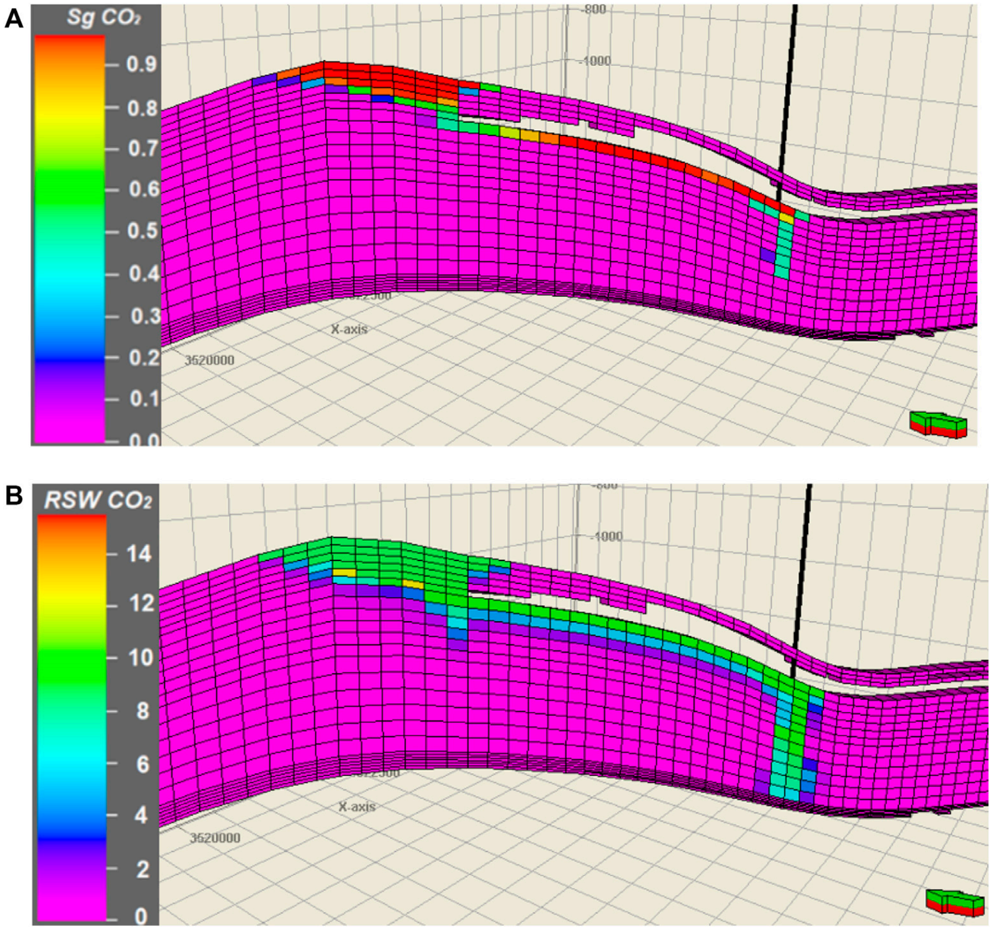

FIGURE 11 | Distribution of free CO_2 saturation in the structure **(A)** and CO_2 dissolved in brine **(B)** after 25 years of injection.

3.3 Simulation Results for Model of Choszczno Structure—Scenario 1

During CO_2 injection simulations for Scenario no. 1 in the Choszczno model, a constant daily injection rate of about 1,449,667 sm^3/d (1 Mt CO_2/year) was maintained. The pressure increase in the sealing roof layers (resulting from the properties and partial penetration of CO_2) was about 5 bar after 25 years of injection. Subsequently, a pressure drop was observed in the tops of the structure resulting from the dissolution of CO_2 in brine. Long-term simulations carried out for a further 1,000 years after the injection has finished showed that when only about 100 years elapsed, the bottom pressure at the top of the structure was merely about 1.5 bar higher than the original pressure before the start of carbon dioxide injection. The bottom pressure in the injection well changes by about 6 bar, whereas the average pressure in the injection zone by about 5 bar (**Figure 6**).

In the case of the simulation of CO_2 injection into the Choszczno structure, similar behaviour of the injected carbon dioxide was observed, i.e., the gravitational migration of CO_2 towards the local top of the structure and simultaneous dissolution of carbon dioxide in brine. However, as mentioned before, the sealing layers in some upper areas of the discussed structure have lower values of clay mineral content (42–60%) than in the rest of the model (above 70%). The permeability of the sealing layers in the upper part of the structure is also high and ranges from 12 to 61 mD. After the simulation, it was found that partial carbon dioxide permeation into the cells of the sealing layers connected to the Pliensbachian collector layers took place. The distribution of CO_2 free saturation in the structure after 25 years of injection is shown in the vertical section (**Figure 9**). In the next Figure, a slow reduction process of the free CO_2 phase can be observed due to the fact that the CO_2 dissolves in brine and falls towards the lower layers of the collector. The distribution of the saturation of the CO_2 dissolved in brine after 25 years of injection is shown in the vertical section by molar fraction (**Figure 9**). In addition, the distribution of the saturation of the carbon dioxide injected in the Pliensbachian collector roof layer (**Figure 10**) and in the roof layer of the reservoir sealing - Toarcian (**Figure 10**) was illustrated.

3.4 Simulation Results for Model of Choszczno Structure—Scenario 2

During simulations of CO_2 injection for Scenario no. 2, a constant daily injection rate of about 2,899 334 sm^3/d (2 Mt CO_2/year) was maintained in the Choszczno model. The bottom pressure in the injection well changes by about 7 bar, while the average pressure in the injection zone—by about 9 bar (**Figure 4**).

Figure 8 shows the comparison of the above-mentioned pressure values for the two injection scenarios. The pressure increase in the sealing roof layers was about 12 bar after 25 years of injection. In comparison, the increase in the same pressure for Scenario no. 1 (injection with a capacity of 1 Mt CO_2/year) was about 5 bar.

In the case of the simulation of the CO_2 injection process with the output of 2 Mt CO_2/year, the rate of carbon dioxide spreading is higher and the size of the area saturated with CO_2 is larger as compared to the results of the simulation of injection with the output of 1 Mt CO_2/year. In a similar way as for Scenario no. 1, the results of the simulations according to Scenario no. 2 for Choszczno structure are presented in **Figures 10**, **11**.

4 CONCLUSION

In this paper, multiple simulations of geological storage of carbon dioxide in brine aquifers of the Choszczno-Suliszewo structure were performed according to the assumed injection scenarios diversified in terms of efficiency. Based on the obtained results of numerical calculations, the changes in pressures characteristic for the sequestration process were analyzed and the spatial distribution of free CO_2 saturation in the structure as well as carbon dioxide dissolved in brine were presented in a graphic form.

During the modelling of the CO_2 sequestration process in aquifers of the Lower Jurassic in the Suliszewo model, the assumed CO_2 injection capacities were achieved for both injection scenarios. As a result of the injection, the pressure rise in the roof part of the collector ranged from 0.5 to 1.0 MPa depending on the injection scenario. The observed increase of pressures does not seem to pose any threat to the tightness of the Suliszewo structure. No changes in pressure in the roof of the reservoir sealing layers were observed in this area.

After carrying out simulations in the Choszczno model, the process of displacement of the injected CO_2 from the collector layers to the layers constituting the reservoir seal was observed. This phenomenon takes place in the upper parts of the Choszczno structure; the locally occurring inferior parameters of seal layers in this region are the main reason for the occurrence of the phenomenon.

An increase in pressure in the roof part of the collector ranging from 0.5 to 1.0 MPa and an additional increase in pressure in the insulating layer of the Toarcian ranging from 0.5 to 1.2 MPa were observed.

In the simulations developed, the formation and gradual development of free CO_2 zones around the injection wells was observed. Another observation was that CO_2 moves towards the collector roof layers and further towards the local top of the structure due to the prevailing buoyancy forces. During the process of the gravitational migration of CO_2 towards the local top of the structure, the phenomenon of the dissolution of carbon dioxide in brine takes place. The longer the gas migration time, the greater is the possibility that CO_2 will dissolve and remain in the pore spaces of the rocks.

A slow reduction of the free phase of CO_2 was observed due to the fact that CO_2 dissolves in brine and falls towards the lower layers of the collector. The brine convection phenomenon occurs due to the changes in its density caused by CO_2 dissolution.

The brine containing the dissolved CO_2 spreads over a much larger area compared to the residual CO_2 zone. The course of CO_2 dissolution in brine largely depends on the effective contact area of carbon dioxide with brine.

The sequestration process was found to be highly effective due to the dissolution of CO_2 in brine and the resulting convective movement of the brine enriched with carbon dioxide. This results in an increase in the sequestration capacity of the structure and permanent long-term trapping of the injected carbon dioxide.

Based on the reservoir parameters of the analyzed structures and the results of numerical simulations carried out, it was found that the Lower Jurassic sandstone formations in the areas in question show very good conditions for the effective underground storage of carbon dioxide.

The simulations performed and the analysis of their results allow to conclude that the CO_2 storage capacity of the analyzed structures significantly exceeds the quantities of the injected CO_2 assumed in the simulations.

It should be noted, however, that there are 19 wells situated up to 30 km from the potential reservoirs in Choszczno and Suliszewo which are relatively easy migration paths for the injected CO_2. Therefore, works preceding the sequestration of carbon dioxide should take into account a detailed study of their technical condition and a possible method of subsequent decommissioning of some wells.

The chemical reaction of CO_2 dissolved in groundwater with groundwater salt solution and rock mineral composition may affect the permeability of CO_2 in the rock formation and in consequence adversely affect the safety of storage. The evaluation of the safety of storage in terms of rock properties are not considered by the authors of this work. Additionally, the results of numerical modeling should be verified after obtaining experimental data of some parameters; for example, the solubility of CO_2 in aqueous solutions of salts. A detailed analysis of the uncertainty of rock properties in the models, the uncertainty of numerical simulation results and sensitivity analysis of model parameters are planned in the framework of additional future work using "Uncertainty and Optimization" module of Petrel software.

DATA AVAILABILITY STATEMENT

The raw data supporting the conclusion of this article will be made available by the authors, without undue reservation.

AUTHOR CONTRIBUTIONS

Conceptualization, TU, JC, MM, and AS; methodology, TU, JC, MM and AS; formal analysis, TU and JC; investigation, TU; writing—original draft preparation, TU, MM, and JC visualization, TU; supervision, AS.

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