CHAPTER 6

USE OF 3D MODELLING IN THE CO_2 GEOLOGICAL STORAGE, POSSIBLE APPLICATIONS FOR PARANÁ AND SANTOS BASINS

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ABSTRACT

The use of 3D modelling in geosciences has become increasingly present in its various applied areas nowadays. This chapter presents a compilation of the international CO_2 storage resource assessment methodologies and their correlation with the use of computational 3D geological modelling techniques currently available through commercial software and open-source alternatives. The applications of these techniques are then discussed concerning the existing spatial data available in the Paraná and Santos sedimentary basins, aiming at assessing possible reservoirs for CO_2 geological storage. The steps from site selection to initial characterization are addressed, including determining storage capacity according to international standards.

Keywords: 3D geological modelling, CO_2 geological storage, Paraná Basin, Santos Basin, CO_2 storage capacity, CCS

1. INTRODUCTION

In the current world climate change scenario where we are experiencing global warming driven by anthropic emissions of greenhouse gases, there is an increasing search for technologies that reduce the planet's average temperature. Many alternatives have been proposed (Lawrence et al., 2018). They include the injection of sulfur dioxide into the atmosphere (Visioni et al. 2017), space-based solar reflectors (Salazar et al. 2016), the covering of deserts, oceans, or grasslands with mirrors that reflect the solar radiation (Salter et al. 2008), ocean iron fertilization (Williamson et al. 2012), and sea spray (Partanen et al. 2012). Among all these alternative technologies, the one that has proven most plausible for implementation in the last few decades is the CO_2 geological storage, including 27 initiatives already in operation presently and more than 62 under development (Global-CCS-Institute 2021). The technology of CO_2 storage integrates a chain of activities that involves trapping the carbon dioxide at its emission source, transporting it to a storage location, and isolating it, named Carbon Capture and Storage (CCS).

The present chapter discusses the use of 3D geological modelling to evaluate potential sites for CO_2 storage, briefly addressing the geological environments currently considered for storage, working scales, and evaluation stages of a given location. The types and techniques of 3D geological modelling presently available are presented and illustrated with some existing examples when possible or with similar applications.

2.3D GEOLOGICAL MODELLING IN GEOSCIENCES

3D geological modelling comprises a group of methods used for computerized representations of any geological body or surface in three dimensions via specialized software, whose final product is generally known as the geological model. 3D geological modelling has a wide range of applications, including but not limited to oil and gas reservoirs, mineral deposits, contamination plumes, groundwater aquifers, nuclear waste underground storage and tunnels, and other underground engineering works. Some examples of application in the oil and gas sector include Bueno et al. (2011); Bigi et al. (2013); Durand-Riard et al. (2013); Aadil and Sohail (2014); Altameemi and Alzaidy (2018); Alhakeem et al. (2019); Trentin et al. (2019); Ali et al. (2020); Palci et al. (2020); Islam et al. (2021). Tectonic approaches through 3D modelling are seen in Brun et al. (2001); Courrioux et al. (2001); Do Couto et al. (2015); de Kemp et al. (2016); Thornton et al. (2018); dos Santos et al. (2019); Lesage et al. (2019); Molezzi et al. (2019).

Some examples of 3D geological modelling supporting mineral exploration are seen in Fallara et al. (2006); de Kemp (2007); Wang et al. (2011); Yuan et al. (2014); Wang et al. (2015); de Kemp et al. (2016); Li et al. (2019); Mao et al. (2019); Wang et al. (2019). 3D modelling applications in a wide range of ore deposits types and geometries can be found in Gumiel et al. (2010); Hill et al. (2014); Vollgger et al. (2015); Basson et al. (2016); Liu et al. (2016); Schetselaar et al. (2016); Pavičić et al. (2018); Stoch et al. (2018); Braga et al. (2019); Xiang et al. (2019); de Oliveira and Sant'Agostino (2020); Arias et al. (2021); de Oliveira et al. (2021a). Applications of 3D modelling on hydrogeology include Artimo et al. (2003); Cox et al. (2013); Hassen et al. (2016); Magnabosco et al. (2020); D'Affonseca et al. (2020). The use of 3D modelling in geothermal reservoirs is presented in Milicich et al. (2010), Milicich et al. (2014), Alcaraz et al. (2015); Poux et al. (2018); Calcagno et al. (2020). Other examples of 3D geological modelling use include the urban and infrastructure areas like Breunig and Zlatanova (2011) and He et al. (2020) and in the differentiation of soils (Queiroz et al. 2017). From this extensive list of references, it is noticed that the application of 3D geological models in several areas of geosciences started to appear more often from the 2000s and grew in recent years. As it is a knowledge area of geosciences in constant expansion due to the recent advances in computer graphics and software technology, there are no limits for new and innovative applications.

A reference book with terms definitions in 3D geological modelling and richly illustrated examples of diverse geological applications is "3D geoscience modelling: computer techniques for geological characterization" (Houlding, 1994). A more recent review of the state-of-the-art geological modelling methods includes Wellmann and Caumon (2018). Other books that also address 3D modelling but are already in some specific geoscience fields are Merriam and Davis (2001) in sedimentary systems, Groshong Jr (2006) in structural geology, Rossi and Deutsch (2013) in mineral resources, and Pyrcz and Deutsch (2014) in oil and gas reservoirs modelling. Perrin et al. (2005) presented a geo-ontology proposal, defining a set of terms for using, sharing, revising, and updating 3D geological models by different users over time. Three special issues of Minerals journal were devoted to the 3D geological modelling theme, "Geological Modelling" (2018); "Geological Modelling, Volume II" (2020); "3D-Modelling of Crustal Structures and Mineral Deposit Systems" (2021). Some specific events and conferences on 3D geological modelling include the workshops held in GSA Annual Meetings, United States (2001, 2002, 2004, 2007, 2009, 2011, 2013, 2015), and in the Resources for Future Generations (RFG), Canada (2018), the European Meetings on 3D Geological Modelling (2013, 2014, 2016, 2018, 2019), and the Visual 3D Conference 2019.

The advantages of 3D geological modelling include expanding the analysis of conventional geological data by visualizing continuities, clusters and spatial trends, geometries of geological bodies or units, structural geological framework, and variation of geochemical contents or any other numerical parameters in geosciences. CO_2 storage models are applied the same way as in oil and gas reservoirs evaluations. They are also used to define suitable reservoir-seal pairs for the trapping of CO_2. It aims to better understand the spatial variability and continuity of the reservoir and seals facies interpretations. The 3D analysis also allowed the ranking of more favourable and unfavourable facies. The main variables from petrophysical wireline logs that can be visualized and estimated in 3D are usually porosity, permeability, and water saturation, considering saline aquifers and depleted reservoirs. In coal seams and shales, the adsorption capacity and total organic carbon (TOC) are important variables of interest.

Some case studies with the specific application of 3D modelling in CO_2 geological storage are present in the literature (Kaufmann and Martin 2008; Douglass and Kelly 2010; Gunnarsson 2011; Monaghan et al. 2012; Alcalde et al. 2014; Lech et al. 2016; Mediato et al. 2017; Shogenov et al. 2017; Vo Thanh et al. 2019; Zhong and Carr 2019). These examples focus mainly on defining the volume capacity to support resource assessment (discussed in the following sections). A different application is the 3D geomechanical model presented by Vidal-Gilbert et al. (2009), which evaluates the changing of in situ stress caused by increased pore pressure during CO_2 injection.

The term geological modelling discussed in this text is not synonymous with numeric modelling, a widely applied technique in geosciences that uses computational simulation to describe the physical conditions of geological scenarios through numbers and equations (Ismail-Zadeh and Tackley 2010). A numeric model could be performed on a grid or a block model with previous domains defined by geological modelling, but this interrelation is not mandatory. The use of numeric models in the CO_2 geological storage is better discussed and exemplified in Chapter 8.

3.3D MODELLING TECHNIQUES

3D geological models may consist of 3D solid surfaces or 3D block models, or both, depending on what features or geological bodies one wants to represent in the three-dimensional space. Generally, the block models are used when the objective is to know some variable in more detail or resolution in a more significant number of points in the space when then estimation, interpolation, or assignments of values are applied to a given block. On the other hand, 3D surfaces are helpful in defining spatial domains, geometries or volumes, and understanding interactions between geological planes. The surfaces or solids generation techniques could be classified as explicit, traditional and implicit modelling (Cowan et al., 2003).

In explicit modelling, the geological interpretation usually comes from polylines drawn directly in 2D projections or digitalized from paper sections with drill holes, wells, geophysical, or any other source of geological data. Generating 3D solids or surfaces requires the polylines to be linked individually and triangulated through tie lines (Fig. 1A). In the implicit modelling, the surfaces to be generated are therefore not constructed directly, as done in the explicit method, but instead are created now from selected points, which could be geological contacts in a well (Fig. 1B). A function is defined throughout space by specifying the function values at selected points and interpolating them through the rest of the space (Cowan et al., 2003). Manual polyline digitization and triangulation in explicit modelling are more labour intensive. These polylines are generated semi-automatically with implicit modelling, allowing automatic updates as new data is available. It is not possible in models consisting of explicit surface triangulations. In some complex cases, the implicit modelling could not be applied as a stand-alone technique, and both of them need to be integrated to get a better result. More in-depth descriptions of these techniques and comparatives can be found in Savchenko et al. (1995), Carr et al. (2001), Cowan et al. (2002); (Cowan et al. 2003; Cowan et al. 2004), Turner (2006), Knight et al. (2007), Birch (2014), Jessell et al. (2014).

Geological contacts and domains could also be defined directly on a block model or grid generating a probabilistic model. In the probabilistic approach, the domains of interest are not defined by surfaces, called meshes or wireframes, representing the geological contacts or faults. Instead, a block model is generated for the studied region. Then, the probability of each block being or not being of a certain lithology or a particular fault side is determined. The probability estimation in each block is performed by geostatistical techniques, commonly indicator kriging, and then by applying threshold values, portions or domains of interest are defined inside the model (Fig. 1C). Geostatistical methods used on categorical variables are better presented, discussed, and exemplified in Journel (1983), Rivoirard (1994), Olea (1999), Lloyd and Atkinson (2001), de Oliveira and Rocha (2011), Pyrcz and Deutsch (2014), Rivoirard et al. (2014).

Several commercial software packages are available nowadays with explicit and implicit 3D modelling engines, as well as geostatistical modules that allow generating probabilistic models, citing: Surpac, Gems, Minesight, Vulcan, Isatis, EarthVision, GeoModeller, Datamine, GoCAD, Leapfrog, Move, Petrel, Micromine, among others. Open-source packages for 3D geological modelling are also available, citing: GemPy (de la Varga et al. 2019; Schaaf et al. 2020); and Loop 3D (Grose et al. 2020; Jessell et al. 2021).

The modelling of the five main geological environments (saline aquifers, oil and gas reservoirs, coal seams, shale, and basalts) where the CO_2 storage has been studied is related to sedimentary basins. The proper characteristics required for CO_2 storage include non-location in the fold and thrust belts and limited to moderate structures (Chadwick et al. 2008; IEA-GHG 2009; Smith et al. 2011). The 3D geological models tend to be more straightforward in these environments. The sedimentary contacts are represented commonly by flat smooth, stacked surfaces. Points generate these surfaces or polylines interpreted from seismic data and the contact points from wells in the subsurface (Fig. 2). The interpretation of distinguished facies with sharped erosional contact could be a challenge for the three-dimension representation due to the complexities involved in the interaction of inter-cutting surfaces. A little bit of complexity may emerge when trying to represent possible fault sets. The most common types are steeply deep normal faults, characteristic of extensional regimes (Etheridge et al. 1985). The fault planes are generated by surface traces interpreted from radar data or satellite images and seismic interpretation.

4. UNCERTAINTY IN GEOLOGICAL MODELLING

Modelling the subsurface geometry is known to be uncertain. Modelling uncertainty is not a goal on its own; usually, it is needed to answer a particular question raised. The subsurface medium's heterogeneity (fluids and soils/rocks) is a critical parameter influencing the decision. Rarely, we have perfect information to model the geological variability of the subsurface deterministically. Hence, there is a need to model all aspects of uncertainty related to subsurface heterogeneity. Several sources of data are available to constrain the models of uncertainty built. These data sources can be remarkably diverse, from wells (driller's logs, well-log, cores, etc.) to geophysical or remote sensing measurements. Tying all this data into a single uncertainty model without making too many assumptions about the relationships between various data sources is quite challenging (Caers 2011).

The traditional geostatistical approach for purposes of uncertainty calculation in geological modelling is carried out, generally, through the sequential simulation of categorical variables, of which stand out truncated Gaussian simulation (Journel and Isaaks 1984; Matheron et al. 1987; Xu and Journel 1993) and the sequential stimulation of the indicators (Journal and Alabert 1989; Alabert and Massonnat 1990). As initially proposed, the sequential simulation's goal is the reproduction of the histogram and the covariance model of the properties to be simulated through the sequential drawing of conditional distributions. Each grid node is randomly visited sequentially, and simulated values are taken from the conditional distribution of value on that node, based on the data neighbourhood and previously simulated nodes. Other examples of simulation techniques used in geological modelling are object-based algorithms or Booleans (Haldorsen and Lake 1984; Stoyan et al. 1987), process-based algorithms (Bridge and Leeder 1979; Lopez et al. 2001), surface-based modelling methods (Xie et al. 2001; Pyrcz and Deutsch 2014) and multi-point simulation algorithms based on pixels (pixel-based) (Guardiano and Srivastava 1993; Strebelle 2002).

5. CO2 STORAGE RESOURCE ASSESSMENT METHODOLOGIES

The classification systems for the assessment stages of a given site for CO_2 geologic storage (Goodman et al. 2011; Rodosta et al. 2011) follow the same processes developed by the petroleum industry (Etherington and Ritter 2008) in a bottom-up progression based on analyses conducted to reduce the project development risk (Fig. 3). Here the application of 3D geological modelling is approached in the Exploration phase, which comprises three stages in increasing order of geological knowledge: Site Screening, Site Selection, and Initial Characterization corresponding to each resource class: Potential Sub-Regions, Selected Areas, and Qualified Site (Goodman et al. 2011; Rodosta et al. 2011). The main technical site selection criteria for geological CO_2 storage (Chadwick et al. 2008; IEA-GHG 2009; Smith et al. 2011) are compiled in Table 1.

6. EXPLORATION PHASE

One of the first parameters to evaluate in any subsurface units suitable for CO_2 geologic storage is a depth of approximately 800 m or more (Chadwick et al., 2008; IEA-GHG, 2009; Smith et al., 2011; Miocic et al., 2016) regarding the CO_2 injected will be in the supercritical condition being in these temperatures and pressures. The CO_2 is stable as a supercritical fluid at a temperature and a pressure above a critical point: 31 ºC and 7.38 MPa, respectively. For these initial appraisals, 3D models of superimposed layers on the formation of interest can be generated on a basin or regional scale from seismic, exploration well, and outcrop data during the Site Screening or Site Selection stages, indicating more or less favourable regions. Similarly, areas with thickness with at least 20 m (Chadwick et al., 2008; IEA-GHG, 2009), caprock thickness with at least 10 to 20 m (Chadwick et al., 2008; IEA-GHG, 2009; Smith et al., 2011), and a safe distance to protected groundwater (IEA-GHG, 2009) could be determined using 3D models. However, in this case, this evaluation would probably occur during the site selection stage since wireline logs with seismic information are needed. A 3D structural model based on seismic data is generated during the site selection stage, indicating possible structural traps favourable for CO_2 reservoirs or areas of less incidence of faults avoiding potential gas leaks (Chadwick et al., 2008; IEA-GHG, 2009; Smith et al., 2011).

The evaluation of whether a basin or portion is located within a fold belt (IEA-GHG, 2009), reservoir-seal pairs, and a favourable stratigraphy (IEA-GHG, 2009; Smith et al., 2011; Miocic et al., 2016) is made at the Site Screening stage. Nevertheless, nothing prevents that with a 3D geological model developed during the assessment advance with new data addition, already in the Initial Characterization stage, the local stratigraphy and structural context may prove more or less favourable, for example, with details of internal facies of a given formation. The addition of a small number of wells or new seismic surveys could dramatically change the interpretation and evaluation of a given area or site.

So we can see that the volumetric evaluation of the CO_2 storage site, where modelling has been applied more frequently (Gunnarsson, 2011; Alcalde et al., 2014; Lech et al., 2016; Mediato et al., 2017; Shogenov et al., 2017; Vo Thanh et al., 2019; Zhong and Carr, 2019), will only occur effectively and commonly in the Initial Characterization stage. Nevertheless, 3D modelling can also be applied in a basin-scale approach at an early stage of exploration (Douglass and Kelly, 2010). An example of 3D geological modelling used in both Site Selection and Initial Characterization stages could be seen in de Oliveira et al. (2021b).

7. SITE CHARACTERIZATION

The U. S. Department of Energy (DOE) methodologies for capacity calculations for the distinguished major geologic media: depleted oil and gas reservoirs, saline formations, unmineable coal seams (Goodman et al. 2011), and organic-rich shales (Goodman et al. 2014) are briefly described next. Other similar volumetric-based methodologies were also developed for CO_2 storage resource assessment (Bachu et al. 2007; Brennan et al. 2010; Bradshaw et al. 2011; Spencer et al. 2011) and were compared and discussed in detail by Popova et al. (2012).

The general equation to calculate the CO_2 storage resource mass estimate for geologic storage in oil and gas reservoirs is based on the standard industry method to calculate original gas or oil-in-place (Dake 1983) as follows:

$$G_{CO2} = Ah_n \Phi (1 - S_w) B \rho_{CO2std} E_{oil/gas} \quad (1)$$

where G_{CO2} is CO_2 mass, A is the area, h_N is the net thickness, Φ is the effective porosity, S_w is the water saturation, B is the initial oil (or gas) formation volume factor, ρ_{CO2std} is the standard CO_2 density, and $E_{oil/gas}$ is the storage efficiency factor, that reflects the volume of CO_2 stored in an oil or gas reservoir per unit volume of original oil or gas in place.

The equation to calculate the CO_2 storage resource mass estimate for geologic storage in saline formations is:

$$G_{CO2} = Ah_g \Phi \rho_{CO2} E_{saline} \quad (2)$$

where h_g is the gross thickness, ρ_{CO2} is the density of CO_2 evaluated at pressure and temperature that represents storage conditions anticipated for a specific geologic unit, and E_{saline} is the storage efficiency factor, reflecting the fraction of the total pore volume that the injected CO_2 will fill.

The equation to calculate the CO_2 storage resource mass estimate for geologic storage in unmineable coal seams:

$$G_{CO2} = Ah_g C_{s.max} \rho_{CO2std} E_{coal} \quad (3)$$

Where $C_{s.max}$ is the maximum CO_2 volume at standard conditions that can be sorbed per volume of coal, assumed to be on an in situ or "as is" basis, and E_{coal} is the storage efficiency factor, which reflects a fraction of the total coal bulk volume that CO_2 contacts.

The equation to calculate the CO_2 storage resource mass estimate for geologic storage in shales:

$$G_{CO2} = AE_A h_g E_h [\rho_{CO2} \Phi E_\Phi + \rho_{sCO2} (1 - \Phi) E_s] \quad (4)$$

where ρs_{CO_2} is the mass of CO_2 sorbed per unit volume of solid rock, and E_A, E_h, E_Φ, and E_S are efficiency factors for the area, thickness, pore-volume, and sorbed volume, respectively (see Goodman et al. 2014 for more details).

Note that all of them use volumetric-based CO_2 storage estimates being computationally equivalent. The volume of a given geological layer *(A x h*), in (1) to (4) equations, can be obtained through the application of the 3D geological modelling techniques presented here with certain precision - depending on the data that support them.

In the present methodologies and the general approach discussed in this text, the 3D models are being considered to use static volumetric models based on commonly accepted assumptions about in-situ fluid distribution in porous media and fluid displacement processes. Currently, most studies are focused on evaluating possible new locations for CO_2 storage. However, 3D geological models can also be used jointly with numerical models, as already mentioned, in the management and monitoring of reservoirs during their injection life (see Chapter 8). A dynamic volume would be considered in this case because detailed site injectivity and pressure data are most commonly available only after CO_2 injection.

When production-based data are available, they should be preferred over a new volumetric-based model estimate in the specific case of an evaluation of depleted oil and gas reservoirs. Production data contain general detailed information collected from the formation.

Similarly to the mineral industry (CRIRSCO 2019) and the oil and gas industry (Etherington and Ritter 2008), for reporting of CO_2 storage capacity, a technical-economic classification system was proposed (Bachu et al. 2007) according to an increasing level of geological knowledge and confidence based on a pyramid (Fig. 4). Storage capacity in this pyramid is expressed in mass CO_2 (e. g., Mt or Gt CO_2) rather than volume because the volume of a given mass of stored CO_2 depends on the pressure and temperature at which it is stored (Bachu et al. 2007). Four technical and economic classes are considered: Theoretical, Effective, Practical, and Matched capacity. A Theoretical capacity assumes that the whole of reservoir formation is accessible to store CO_2, providing a maximum upper limit to a capacity estimate. The application of technical constraints as cut-off limits of porosity and permeability, and limiters as seal quality, depth of burial, pressure and stress regimes, the reservoir's pore volume, and trap determines the Effective capacity. The practical capacity considers economic, legal, and regulatory barriers to CO_2 geological storage beyond just geoscience and engineering aspects. It corresponds to the reserves used in the petroleum and mining industries.

The Matched capacity refers to the detailed matching of significant stationary CO_2 sources with adequate geological storage sites considering potential, injectivity, and supply rate. Other refinements and modifications of the initial pyramid have been proposed recently (Ackhurst et al. 2011; Bunch 2013; Anderson 2017; Vasilis et al. 2018; Mikhelkis and Govindarajan 2020), although all considering a decrease in the geological and economic uncertainty of the classes from the bottom to the top.

Most mineral resource and ore reserve classification systems adopted are based on sampling spacing, geological confidence, and economic viability. These systems define categories of resources based on a degree of uncertainty associated with parameters being estimated. Evaluation and classification are included in the mineral resource and CO_2 geological storage sites assessment. Drilling and sampling combined with quality assurance and quality control practices systematically update this process. New and sophisticated methods used for modelling and evaluation are worthless if sampling, preparation, and chemical assays are not adequately controlled and validated. The procedure selected for the CO_2 geological storage sites classification should have some required characteristics. The method used for classification should be able to define confidence either in geometry or petrophysical properties estimates. Classes of storage sites are determined based on the sample's spatial distribution and the uncertainty associated with tonnages calculated for a given deposit or part of it. Thus, the classification of a mineral resource requires the definition of the uncertainty associated with the estimate. However, what is not clearly stated in the main classification systems is how uncertainty should be assessed.

8. DATASETS FOR CO_2 STORAGE RESOURCE ASSESSMENT

Generating a model representing some geological form or body depends on previous georeferenced data in three dimensions. Georeferenced data is any geological data or information that has spatial coordinates X, Y and Z defined. These data can be of land surface topography, maps, drill holes or wells, geophysical surveys, location points of outcrops, structural measures, samples, among others. Therefore, the first step to evaluate before starting the geological modelling is to check what data is available for the area of interest and if it is possible to use them in a 3D environment. More details about data types and methodology for an integrated 3D model could be seen in Kaufmann and Martin (2008). All GIS data presented in the figures 5 and 6 is public data and come from Agência Nacional do Petróleo, Gás Natural e Biocombustíveis, Brazil (ANP) (http://geo. anp. gov.br/)

and from Companhia de Pesquisa de Recursos Minerais, Brazil (CPRM) (http:// geosgb. cprm. gov.br/).

9. AVAILABLE DATA FOR PARANÁ BASIN

The Paraná Basin presents CO_2 storage potential to be investigated in almost all types of CO_2 geological storage: saline aquifers and coal seams (Rio Bonito Formation), shales (Irati Formation), and basalts (Serra Geral Formation). Some of these geological environments already had some preliminary work. The saline aquifers hosted in Rio Bonito Formation were initially focused, and experimental studies suggested that CO_2 could be permanently stored as carbonates due to good reaction with host rocks (Ketzer et al. 2009; Lima et al. 2011). The Rio Bonito Formation also presents depth and thicknesses compatible with storage approximately CO_2 stationary sources (Rockett et al. 2011; Machado et al. 2013). The CO_2 sorption capacities were initially assessed on coals from the Rio Bonito Formation and oil shales from Irati Formation with potential for storage and coalbed methane production (Weniger et al. 2010; Kalkreuth et al. 2013; Santarosa et al. 2013). The Irati Formation shales were addressed on CO_2 storage investigations considering a possible shared production of methane (Mabecua et al. 2019; Richardson and Tassinari 2019; Rocha et al. 2020).

The Paraná Basin presents an extensive data set with 123 hydrocarbon exploration well data. Petrobras Company carried out this survey from the 1950s until the 2000s, with more than 61,100 line kilometres of 2D reflection seismic data covering most of its extension (Fig. 5), and local electromagnetic, magnetic, and gamma surveys, as well as geological maps in regional scale. These data allow the interpretation of the main layers of interest of Irati and Rio Bonito Formations, delimiting units and facies within these formations, and evaluating depths, thickness, distance from protected groundwater. These were used to interpret structures and traps for storage, allowing further capacity calculations and economic evaluations using 3D geological models.

10. AVAILABLE DATA FOR SANTOS BASIN

The potential for CO_2 storage in the Santos Basin is verified, especially from the study of the oil and gas fields in its extension, which is justified by the less accessible nature of offshore basins. The reuse of oilfield infrastructures and the geological knowledge associated with these enterprises favours that the optimal environment for storage is the natural structure of the oil reservoirs.

Therefore, the use of depleted fields for storage in the Santos Basin seems a natural path because it results in lower costs, less environmental damage, and more excellent local geological knowledge (Hannis et al., 2017). The Santos Basin has eight exploratory plays in its extension, and throughout its territory, there is robust coverage of seismic surveys. Therefore, when associated with oil reservoirs, the target formations for storage in the Santos Basin are those that correspond to the reservoir rocks: Marambaia Formation, Santos Formation, Juréia Formation, Itajaí-Açu Formation, Guarujá Formation, Florianópolis Formation, Itanhaém Formation (Freitas et al. 2006; Moreira et al. 2007; Chang et al. 2008). Turbiditic sandstones of the Upper Cretaceous are the focus for CO_2 storage. The pre-salt reservoir formations are not considered because their very high depths diverge from the optimum characteristics for CO_2 storage. An initial CO_2 storage evaluation on Santos Basin considered the Merluza zone indicating geological favorability and the presence of installed infrastructure that can be reused after adaptations (Ciotta and Tassinari 2020). Another potential that could be explored in Santos Basin is the anthropic excavation of salt caverns in ultra-deepwater (da Costa et al. 2019a; da Costa et al. 2019b; Goulart et al. 2020). The selection of a cluster of salt domes for the location of the first experimental and pilot caverns built-in ultra-deepwater was based on interpretation of 3D seismic and 2D seismic from one of the major pre-salt oil fields in Santos Basin (Goulart et al. 2020).

The basin has 27 oil fields, five non-associated gas fields, and eight fields under evaluation. The data collection resulting from the Santos basin's exploratory efforts includes 435 exploratory wells, a dense mesh of seismic data, and 3D seismic surveys that cover a large part of the basin (Fig. 6). The availability of this data allows an in-depth study of the viability of the Santos Basin fields for storage. Thus, it is possible to verify the essential characteristics of a CO_2 sink (e. g., depth, thickness, integrity) and the verification of the long-term permanence of the gas from the verification of the adjacent formations. The availability of these data also enables the production of reservoir models, favouring understanding the fluid dynamics at the sites of interest and a scale prediction of storage capacity.

11. FINAL CONSIDERATIONS

The chapter brings a brief review of some applied examples of 3D geological modelling in geosciences in the last years, focusing on CO_2 geological storage. International CO_2 storage resource assessment methodologies are presented and discussed, in the stages, when the 3D modelling could be useful and expected results. Since all assessment methodologies proposed to the current use volumetric-based

CO_2 storage estimates, the site characterization phase is when the 3D modelling is presented to be used for the volume and posterior capacity calculation. However, there are still few examples in the literature. Nevertheless, there is an excellent variety of 3D modelling applications in the Exploration phase, such as thickness models for the reservoir formation and the depth seal rock, favourable depth models, and distance models for protected aquifers. The 3D ambient could also help integrate distinguishing data from the surface, seismic and other geophysical surveys, wells, and derived data, helping select favourable areas or sites.

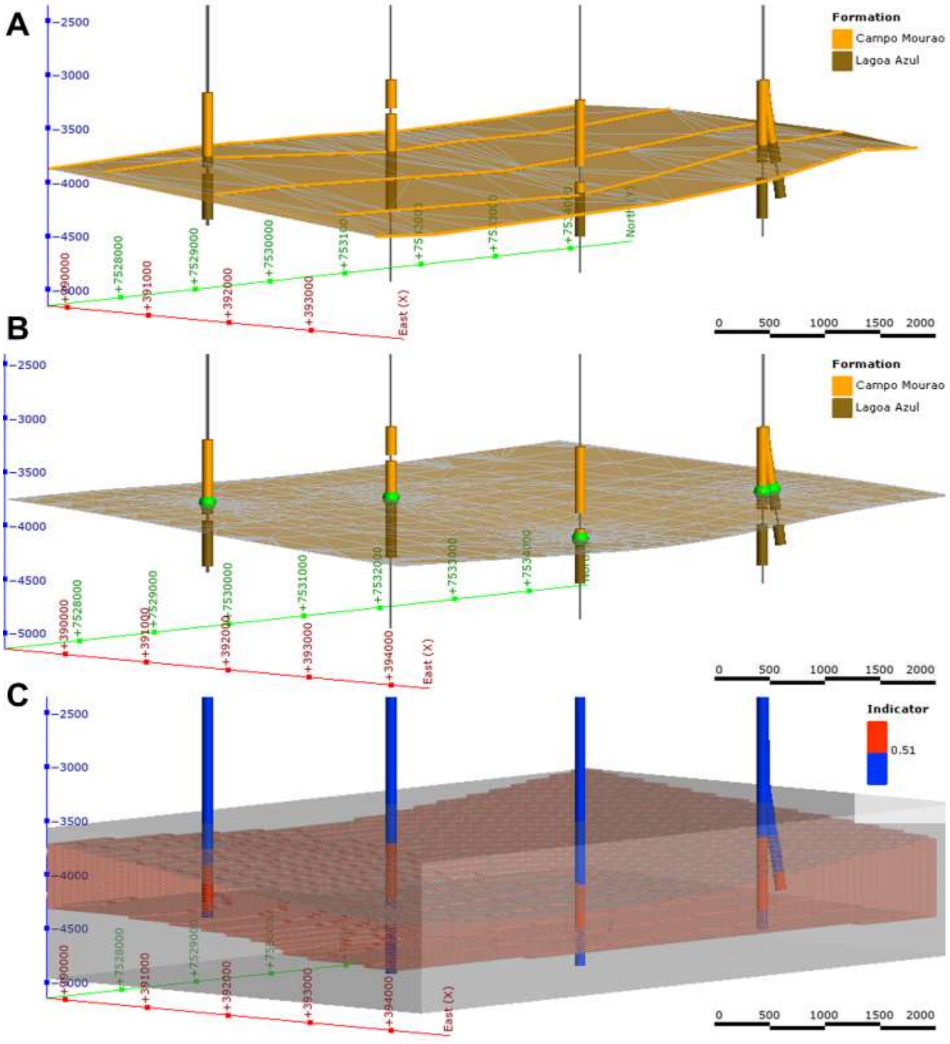

Fig. 1. Comparison between different 3D geological modelling techniques for an example of the contact between sedimentary layers. A) Explicit modelling, B) Implicit modelling, C) Probabilistic modelling

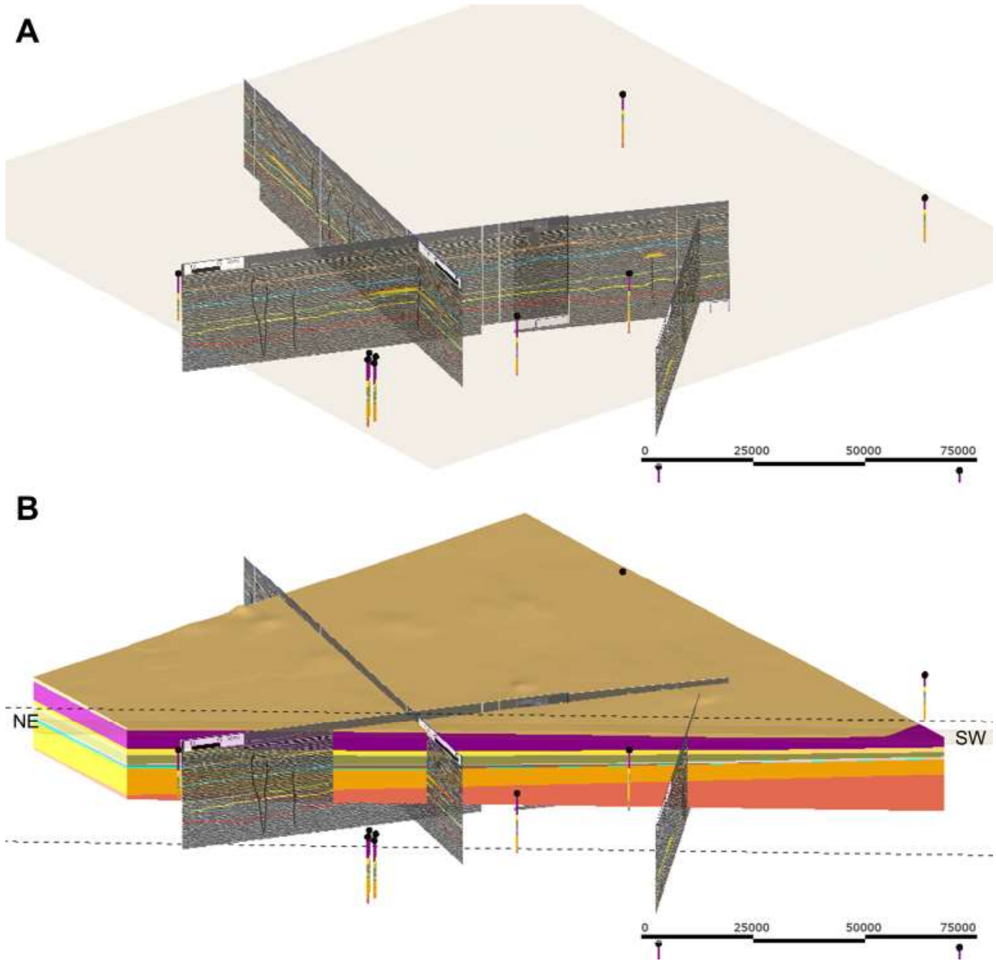

Fig. 2. A) Example of data integration of topography surface, interpreted seismic sections, and exploration well data in a 3D environment. B) 3D stratigraphic model generated from the data together.

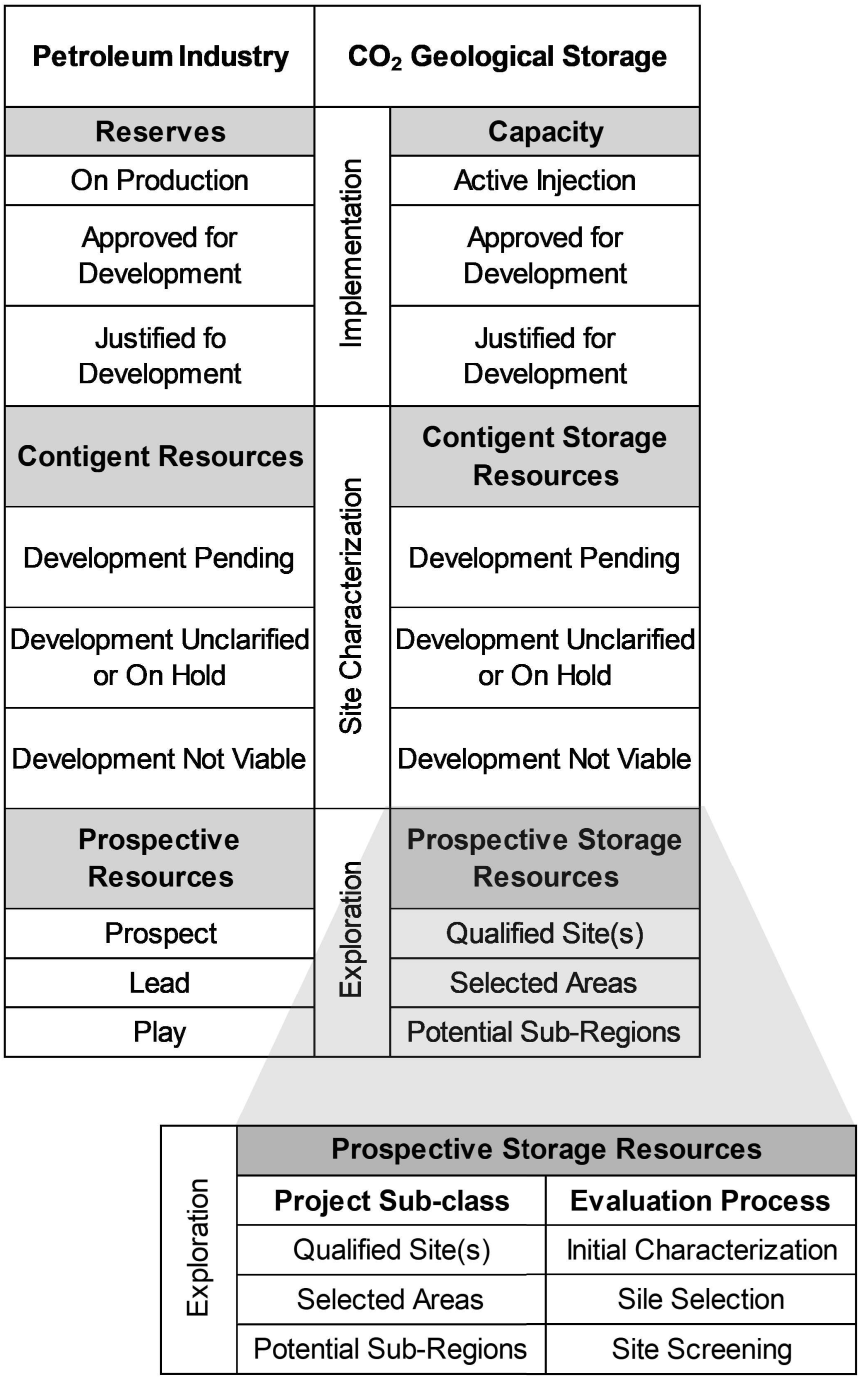

Fig. 3. CO_2 geologic storage classification system (after Goodman et al. 2011)

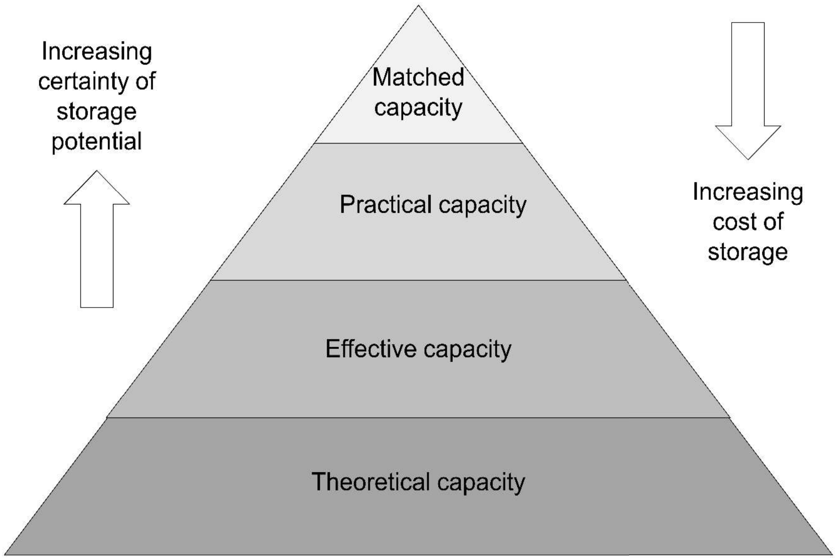

Fig. 4. Techno-economic resource pyramid for capacity for CO_2 geological storage (after Bachu et al. 2007).

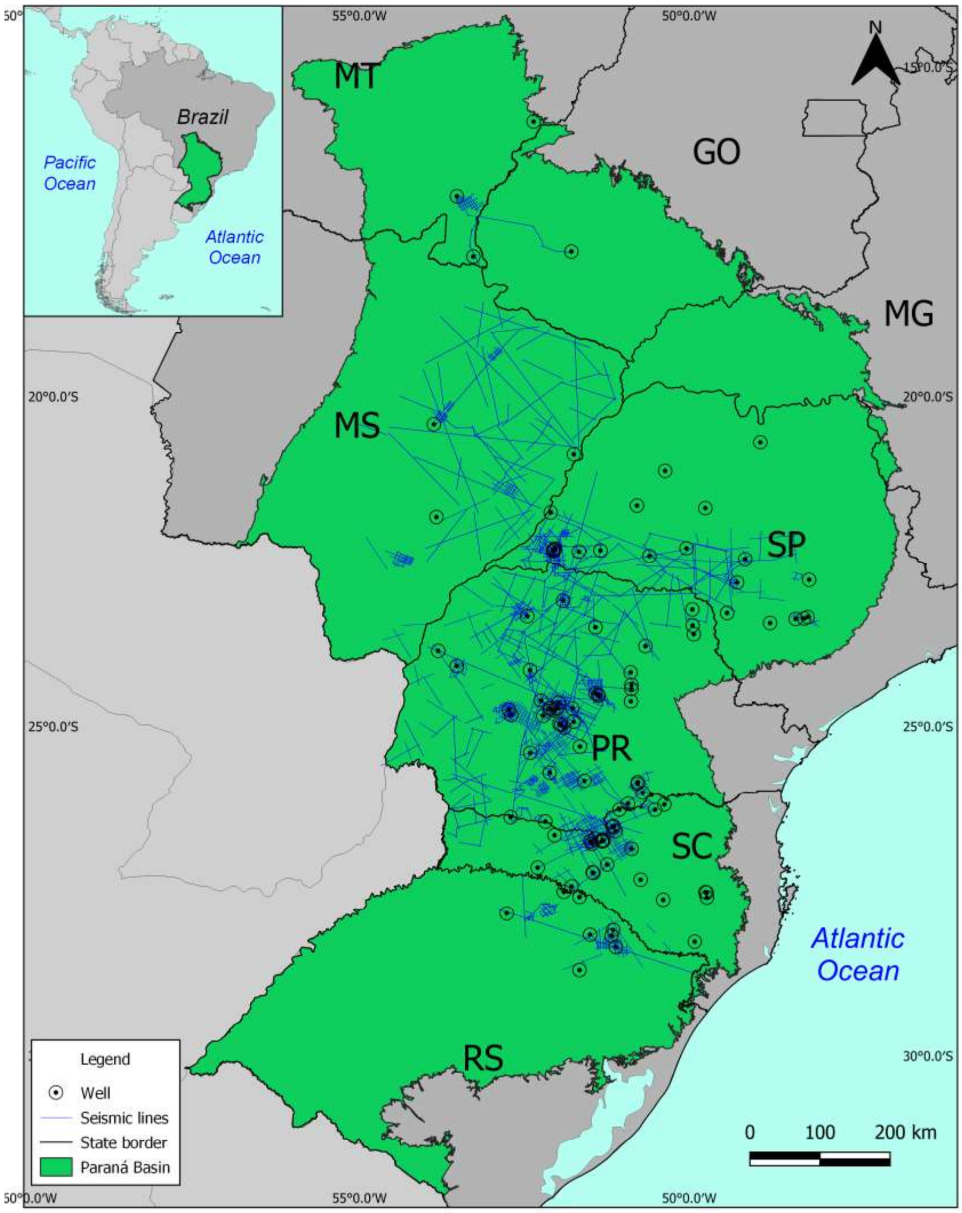

Fig. 5. Available data of seismic and exploration wells for Paraná Basin (data from ANP, 2021)

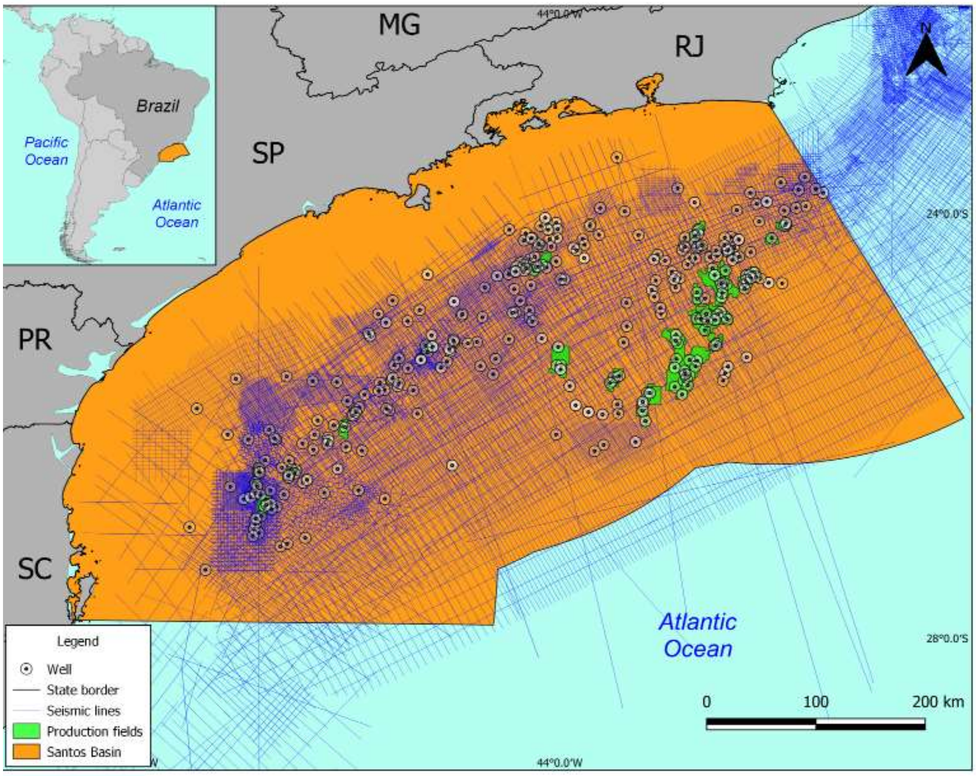

Fig. 6. Available data of seismic and exploration wells for Santos Basin (data from ANP, 2021)

Criterion	Eliminatory or unfavourable	Preferred or Favourable	References
Reservoir-seal pairs; an extensive and competent barrier to vertical flow	Poor, discontinuous, faulted and/or breached -	Intermediate and excellent; many pairs (multi-layered system) Vertically sealing faults, multi-layered systems	IEA-GHG, 2009 Miocic et al., 2016
Stratigraphy	Complex lateral variation and complex connectivity	Uniform	Smith et al., 2011
Located within fold belts	Yes	No	IEA-GHG, 2009
Depth	< 800 m or > 2,500 m < 750-800 m < 800 m > 2,500m -	Between 1,000 and 2,500 m > 800 m > 800 m < 2,500 m > 1,200 m	Chadwick et al. 2008 IEA-GHG, 2(IEA--GHG 2009)009 Smith et al., 2011 Miocic et al., 2016
Thickness	< 20 m < 20 m	> 50 m ≥ 20 m	Chadwick et al. 2008 IEA-GHG, 2009
Affecting protected groundwater quality	Yes	No	IEA-GHG, 2009
Faulting and fracturing intensity	Extensive	Small or no faults Limited to moderate Minimal faulting, with a trapping structure	Chadwick et al. 2008 IEA-GHG, 2009 Smith et al., 2011
Caprock thickness	< 20 m < 10 m < 20 m thick -	> 100 m ≥ 10 m > 100 m thick > 150m	Chadwick et al. 2008 IEA-GHG, 2009 Smith et al., 2011 Miocic et al., 2016
Lateral continuity of caprock	Lateral variations faulted	Unfaulted (uniform)	Chadwick et al. 2008
Total storage capacity	Total capacity is estimated to be similar to or less than the total amount produced from the CO_2 source	Total capacity is estimated to be much larger than the total amount produced from the CO_2	Chadwick et al. 2008

Table 1. Compilation of site selection criteria for geological CO2 storage where 3D geological modelling could be applied.

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