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Carbon Dioxide Geological Storage (CGS) – Current Status and Opportunities

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Abstract

Carbon dioxide sequestration has gained a great deal of global interest because of the needs and applications of mitigation strategy in many areas of human endeavors including capture and reduction of CO₂ emission into atmosphere, oil and gas enhanced production, and CO₂ geological storage. In recent years, many developed countries as well as some developing ones have extensively investigated all aspects of the carbon dioxide geological storage (CGS) process such as the potential of storage sites, understanding the behavior of CO₂, and its interaction with various formations comprising trapping mechanisms, flow pattern, and interactions with formation rocks and so on. This review presents a summary of recent research efforts on storage capacity estimation techniques in most prominent storage options (depleted oil and gas reservoir, saline aquifers and coal beds), modeling and simulation means followed by monitoring and verification approaches. An evaluation of the more interesting techniques which are gaining attention in each part is discussed.

Keywords: carbon dioxide, geological storage, CGS

1. Introduction

Carbon dioxide (CO₂) is one of the most emitted greenhouse gases (GHG) which causes heat trapping of the earth and contributes to the global climate change. This global issue led to the public concern and has become a serious problem in the developed and developing countries [1]. Accordingly, the increase of GHG in the atmosphere has led to a rise in the average global temperatures with a warming forecast of 1.8–4.0°C [2]. Recent surveys conducted, see [2–5], show that the CO₂ concentrations has risen from pre-industrial levels of 280 parts per million (ppm) to present levels of ~380 ppm in the atmosphere and this increase in CO₂ concentration depends on world's expanding use of fossil fuels. Further studies, according to the CO₂

emissions from fossil fuel power plants, represent the amount of emissions around 23 Gton- CO_2 per year and 26% of the total emissions approximately [1, 2, 6]. Reports from on-road transportation emissions also indicate the high contribution of CO_2 in atmosphere especially in urban areas. It contributes around 10% of the total global and 20% of the European atmospheric CO_2 emissions [7]. Based on the Intergovernmental panel on Climate Change (IPCC) report in 2005, 72% of the anthropogenic greenhouse effect is due to the CO_2 emission and it is considered as the most important GHG contributor [1]. The Kyoto Protocol in 1997 also recommends that the nations minimize their CO_2 emissions up to 95% of 1990 levels by 2012. In this regard, the mitigation options of the CO_2 have been defined in many national and international scales and the scientists have been looking and developing for the techniques which reduce the CO_2 emissions [8–11]. The options include reduction in using carbon-intensive fuels and improving energy efficiency in order to decrease the CO_2 emissions into the atmosphere or carbon sequestration.

CO_2 sequestration is the process of injecting CO_2 into sub-surface to reduce the emissions of anthropogenic CO_2 . According to the IPCC 2005, the storage options are classified into three groups: (1) ocean storage, (2) mineralization, and (3) geological storage. Ocean storage consists of injecting the CO_2 into deep oceans and immobilizing it by dissolving or forming a plume which is heavier than water under the ocean. The ocean is the largest storage option of CO_2 and can contain 40000 Gton of carbon in contrast to the 750 Gton in the atmosphere. The ocean storage has not yet been considered as a pilot scale since it is still in the research phase and may also have dire consequences in marine life in case of leakage during and after the storage. [1, 12]. Mineralization process provides an opportunity to store the CO_2 for a long period of time without any special concern about the permanent mitigation quality. It includes the CO_2 conversion to a solid inorganic carbonates which is stable for a long time. The only considerable problem in this process is related to the high cost of implementation [13]. The CO_2 geological storage (CGS) is considered as the main process for CO_2 sequestration in the developed world [14–16]. The candidate CO_2 storage facilities consist of deep saline aquifer and unmineable coal deposits, as well as depleted and mature oil and gas reservoirs which can contain 2200 Gton of carbon dioxide [17]. Based on an estimation reported by the European technology platform for zero emission fossil fuel power (ZEP), the contribution of each option for the storage potential of CO_2 is shown in Figure1. [18]

As for CGS's regulation in Europe in 2009, the European Union approved that seven million tons of CO_2 could be stored by 2020 and up to 160 million tons by 2030, assuming a 20% reduction in GHG emissions by 2020 [19]. Over the past decade, many developed countries have extensively investigated the potential of CO_2 storage sites as well as understanding the behavior of CO_2 and its interaction with different reservoir formations as a prerequisite to increase the effectiveness and integrity of the CGS projects. These comprise advanced scientific knowledge about CO_2 behavior such as trapping mechanisms (physical and chemical), flow patterns, and interactions with formation rocks that can be achieved by improved techniques such as flow simulation, reservoir modeling, reservoir monitoring, and verification [20].

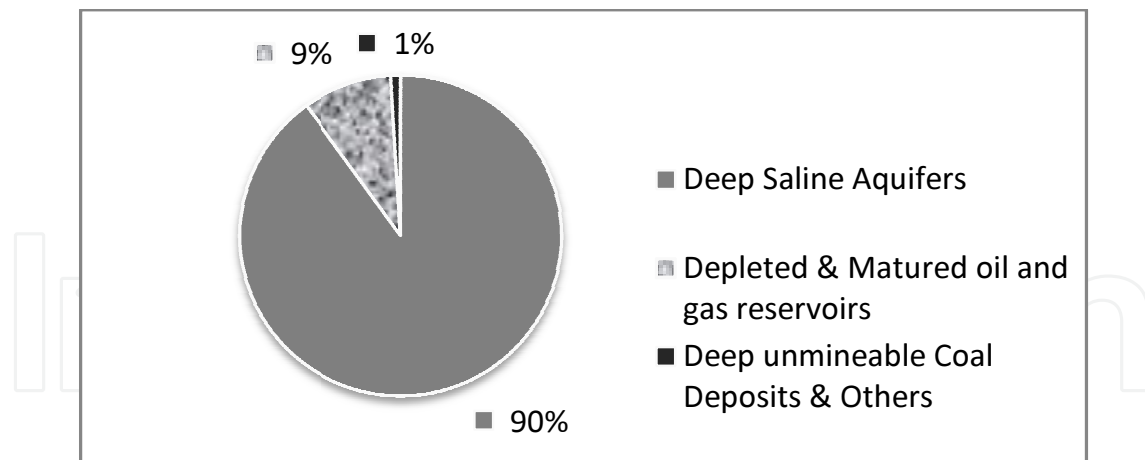


Figure 1. The contribution of most important CGS techniques in the world's CGS projects.

2. CGS: Storage Capacity

In recent years, there have been a number of surveys related to the storage capacity estimation methods in CGS fields [21]. The first groups of estimation assessments were simple with no technical component similar to the estimations held in Europe by Holloway and van der Straaten, in 1995, while the other recent ones have taken into account the complexities and more sophisticated methods of estimating the CO₂ storage capacity [22–28]. One should keep in mind that the capacity estimation in any different scale (global, reservoir, basin, or region) and time frame is a difficult process due to our lack of knowledge about subsurface in most areas of the world and also the uncertainties and inaccessibility of the available data [29]. However, there is a wide variety of estimation techniques proposed by different authors (CSLF, IPCC, and Bradshaw et al.) which mainly rely on a simple algorithm depending on various storage mechanism [26, 28, 30].

In 1979 and 1988, the concept of resource pyramids was developed by Masters and McCabe for the first time and was later proposed to demonstrate the accumulation and quality of the CO₂ storage potentials in the form of three pyramids as an important factor for capacity estimation, including (1) high level, (2) techno-economic, and (3) trap-type and effectiveness pyramid [31, 32]. This concept consists of the main aspects of CO₂ storage such as different time scales and assessment scales, various assessment types, and different geological storage options [29]. For instance, as it has been demonstrated in Figure2, the techno-economic resource pyramid calculates the storage capacity in mass instead of the volume and includes the maximum upper limit of capacity estimate with various time and assessment scales. On the other hands, it reveals three levels of theoretical, realistic and viable estimates in which the theoretical portion includes the entire pyramid whereas the realistic and viable parts have covered the top two portions and only the top portion of pyramid respectively [28, 30].

In an investigation which was performed by Kopp et al. in 2009, to estimate the effective storage capacity, some models were proposed by authors, including(1) CSLF model (proposed by Bachu et al. in 2007 in which the effective storage volume is calculated by reducing the capacity

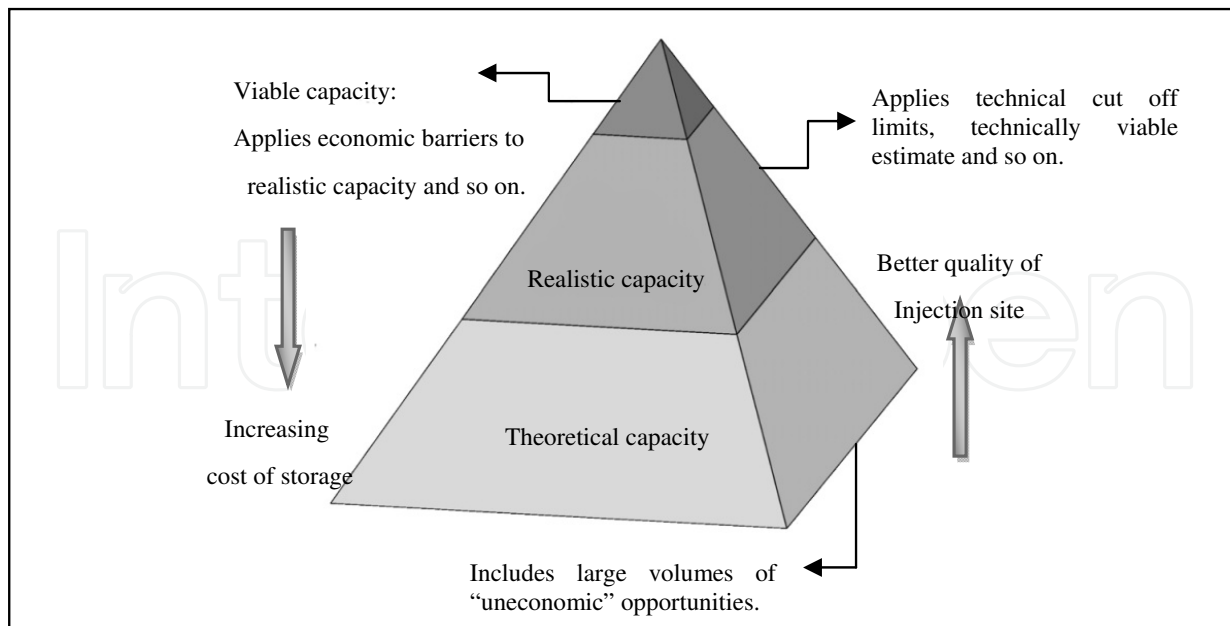


Figure 2. Techno-Economic Resource Pyramid for capacity estimation in CO₂ geological storage.

coefficient from theoretical capacity), (2) Doughty model (proposed by Doughty et al. in 2001 which estimated the effective capacity as a volume fraction for CO₂ storage), and (3) Kopp model (based on Doughty model while the pores containing dissolved CO₂ is much larger than those containing free gas [33]).

According to CO₂ storage capacity estimation surveyed by Bachu et al., based on a summary of carbon sequestration leadership forum (CSLF), different timeframes and field scales are accounted considering various trapping mechanisms (physical and chemical mechanisms) [26]. Bachu et al. have demonstrated the approaches based on different geological potential with generally assessing the opportunity of other storage options like man-made underground cavity and the basalts such as Deccan Plateau in India; however, they need more investigations.

2.1. Estimation techniques in depleted oil and gas reservoir

DOE (2006), 'Methodology for development of carbon sequestration capacity estimates' and CSLF (2007), 'Estimation of CO₂ storage capacity in geological media – phase II' are the major investigations regarding the storage capacity estimation approaches in geological formations. The CSLF (2007) employs a techno-economic resource pyramid in the capacity estimation process for depleted oil and gas reservoir based on McCabe (1998), while the DOE (2006) utilizes volumetric equations and Monte Carlo approach to estimate the uncertainty and capacity storage by incorporating various trapping mechanisms in depleted oil and gas reservoirs [31]. Another integration of DOE and CSLF with simple version of SPE (Society of Petroleum Engineering) petroleum resource management system is proposed and called CO₂CRC storage capacity classification [34, 35]. They have reported that on account of greater amount of data in term of oil and gas fields, the estimation process is the easiest among the

geological formations. It should be noted that the other methods which are employed in saline aquifers can be used here for CO₂ storage volume estimation: 'volumetric-based estimation' and 'production-based estimation' [35, 36].

Bachu et al., provided a good overview of storage capacity estimates in oil and gas reservoirs to compare the other geological formation such as coal beds and saline aquifers [26]. Based on Bachu et al., the capacity estimation in oil and gas reservoirs is more convenient than other geological formations, and these geological formations are discrete in contrast to the continuous coal beds and saline aquifers [26]. Estimation of the CO₂ storage capacity is also difficult for a number of reasons: In estimation process, some assumption would be made, such as volume occupied by hydrocarbons is available for CO₂ after production for pressure-depleted reservoirs with no hydrodynamic contacts. On the other hand, formation water influx as the consequence of pressure decline and water trapping can be inverted due to the CO₂ injection and increase in the pore spaces which may cause some pores to be unavailable for CO₂ storage. Thus, the original reservoir pressure has the maximum limitation for CO₂ injection into the depleted reservoirs [37]. According to the volume of original oil and gas at surface conditions, theoretical mass storage capacity can be accounted through an equation proposed by Bachu et al. [26]. They also provided an extrapolation to account the theoretical storage capacity in another correlation. In some cases, the actual volume availability to CO₂ storage can be reduced and would be stated by capacity coefficient (equation expressed by Doughty and Press, 2004) [38]. But based on Bachu and Shaw, in 2005, enough data are not available for assessing these coefficients, and estimations are mostly carried out by numerical simulations [9, 38]. One of the specific issues in CO₂ storage in depleted reservoirs is CO₂ flood-enhanced oil recovery. Because of some reasons, the capacity estimation in this case is already an effective estimation. The promising storage sites for CO₂ enhanced recovery can be performed at regional and basin scales such that this criterion decreases the effective capacity to practical storage capacity [39–41].

2.2. Estimation techniques in saline aquifers

As it has been illustrated in recent studies, deep saline aquifers are the most favorable storage option in comparison to the depleted reservoirs and coal beds [1, 27, 28, 39]. In contrast, the numbers of projects which have been conducted by the industries are not considerable due to some reasons, including availability of anthropogenic CO₂ and the related data, site assessment difficulties, poor injectivities, and high cost of monitoring [42]. According to the DOE, a volumetric equation is proposed to CO₂ storage estimation in saline aquifers, while each type of trapping mechanisms is also needed for calculation of the basin-scale assessments [35]. In CSLF methodology for deep saline aquifers, storage estimations based on structural and stratigraphic trapping mechanisms are similar to depleted oil and gas reservoirs, whereas the mass of CO₂ related to the effective storage volume would be more difficult to calculate. Moreover, the storage estimation based on solubility trapping at the basin and regional scales can be calculated by the relation proposed by Bachu and Adams [36, 41].

Bachu et al. proposed a theoretical approach to CO₂ storage estimation considering each type of trapping mechanism in deep saline aquifers [26]. They introduced a simple time-independ-

ent volumetric equation used for depleted oil and gas reservoirs in which the traps have been saturated by water rather than being occupied with hydrocarbons. Similar to equation mentioned above, a relation related to the CO₂ mass storage limitation also has developed here for basin- and regional-scale assessments, which can be utilized for theoretical and effective capacity estimations. For residual gas trapping method, the storage volume can be calculated with a time-dependent equation proposed by the authors with regard to the concept of actual CO₂ saturation at flow reversal by Juanes et al. [43]. The solubility mechanism is a time-dependent, continuous, and slow process which can be performed effectively after finishing the injection process. If this trapping system occurs in thick and high permeable aquifers, a convection cell can be constituted and the dissolution process will be improved, while in the case of thin aquifers, this mechanism is less efficient [44, 45]. Capacity storage at the basin and regional scale can be assessed through an equation proposed by Bachu and Adams whereas at the local and site scale, numerical simulation is required for precise estimation of the storage capacity [41]. Estimation through mineral trapping cannot be applied at the regional and basin scales due to the lack of available data and the complex intrinsic of mineral trapping and the chemical and physical related mechanisms. The only remaining approach is numerical simulation which is suitable for site and local scale during a long period of time. According to recent research, mineral trapping mechanism can be compared to the solubility mechanisms with regard to the long time period required here [46, 47]. Hydrodynamic trapping mechanism consists of all the mentioned features of the mechanism and it needs various time scales for acting. This process cannot be evaluated at regional and basin scale estimations due to the different acting time scales through various trapping mechanisms. Hence, it should be considered in a specific point of time and the numerical simulation applied to estimate the storage capacity at local and site scales [26, 48].

De Silva and Ranjith conducted a complete investigation related to the CO₂ estimation methods on saline aquifers and assessed different aspects of the estimation process such as operating time frame, resource circles (pyramids), and trapping mechanisms and factors affecting the storage capacity [50]. The proposed equations in each trapping system are based on the relations recommended by Bachuet al. [26]. The evaluated parameters which can affect the storage capacity consist of *in-situ* pressure, injectivity, temperature, permeability, and compressibility. According to De Silva and Ranjith, eight methods have been introduced to estimate theoretical and effective capacity of CO₂ storages (volumetric method, compressibility method, flow simulation, flow mathematical models, dimensional analysis, analytical investigation, Japanese methodology, and Chinese methodology), while to calculate the practical and matched capacities, the local conditions need to be considered [26, 49, 50]. In a quick and simple volumetric method, the porosity, area, thickness, and storage efficiency of the storage reservoirs are important in capacity estimation according to an equation mentioned by DOE and Ehlig-Economides and Economides [see 51, 52], while van der Meer and Yavuz have proposed another equation to measure the CO₂ mass [53]. To calculate the volume of CO₂ per volume of the aquifers, Eccles et al. have introduced another relation including measuring the effective capacity storage at a special depth [54]. The more comprehensive equation to calculate the storage capacity by compressibility method was shown by

Zhou et al. [55]. The most effective method to assess the capacity is the flow simulation which includes volumetric formulas and more reservoir parameters rather than other methods [56]. Mass balance and constitutive relations are accounted in mathematical models to capacity assessment and dimensional analysis consists of fractional flow formulation with dimensionless assessment and analytical approaches [33]. From the formulations demonstrated by Okwen and Stewart for analytical investigation, it can be deduced that the CO₂ buoyancy and injection rate have affected the storage capacity [57]. Zheng et al. have indicated the equations employed in Japanese and Chinese methodology and have noted that some parameters in Japanese relation can be compared to the CSLF and DOE techniques [58].

2.3. Estimation techniques in coal beds

According to the IPCC 2005, the coal bed storage process is currently in the demonstration phase. MacDonald of Alberta Energy reported the storage in coal bed in 1991 for the first time [59]. One of the most prominent factors to guarantee the successful economic CO₂ storage process is the permeability of coal and it should be more than 1 mD (miliDarcy) [60]. The main problem in CO₂ storage in coal bed process is the limitation of available data about location and capacity of promising sites [30, 26, 28]. It should be noted that the main trapping mechanism in storage process regarding the coal beds is adsorption, and it is necessary to assess the rank, grade, and type of the coal in order to achieve more information about adsorption capacity of the coals [35].

The CSLF and DOE proposed models such as volumetric equation to estimate the coal capacity through substituting the intrinsic methane by injected CO₂ process. Bachu et al. have reported the relation demonstrating the initial gas in place after coal adsorption process proposed by van Bergen et al. and White et al. [59, 61, 62]. One should keep in mind is that since the adsorption is one of the main parts of the storage process, adsorbed gas capacity estimation is also important to investigate [63]. Langmuir equation is a simple and efficient relation for single-layer adsorption capacity estimation in low-pressure conditions [64–66]. In case of high pressure and high temperature, other methods are more suitable such as Bi Langmuir, extended Langmuir, Sips, Langmuir-Freundlich, Toth, UNILAN, two-dimensional EOS, LRC (loading ratio correlation), Dubinin-Radushkevich (D-R) and Dubinin-Astakhov (D-A) [59, 67–73]. A modified Langmuir and Toth correlation was expressed by Himeno et al. and Bae and Bhatia, which includes the substitution of pressure by fugacity high dense phase conditions [74, 75]. Another mathematical power equation proposed by Saghafi et al. can be used to estimate the adsorption capacity [66].

Storage capacity estimation for the stored gas content can be performed through the equation suggested by White, van Bergen et al., CSLF, and Vangkilde et al. [61, 76, 77]. Palarski and Lutynski expressed another relation to estimate the CO₂ storage components in coal seams [78]. To estimate the large-scale storage capacity of 45 important coal basins during Enhanced Coal Bed Methane Recovery (ECBM) in China, Li et al. used an equation which can be modified to a simpler form without considering the different coal bed basins [63, 79].

3. CGS: Modeling and Simulation

To study the behavior of CO₂ during and after the CGS process, numerical modeling is considered as the only effective tool prior to the experimental and field demonstrations instead of analytical and semi-analytical solutions on account of some limitations and simplifications [80–83]. In the past few years, various numerical modeling and reservoir simulations approaches have been documented in the literature at the pilot and commercial scales which are using common numerical methods such as finite difference, finite element, and finite volume methods. One of the most efficient means for reservoir modeling is TOUGH2 simulator developed by Pruess et al. and used successfully in Rio Vista reservoir. In this study, an extension of EOS7R and EWASG modules have been developed to simulate the gas and water flow called EOS7C [84–88]. Omambia and Li carried out a CO₂ numerical modeling in a deep saline aquifer (Wangchang basin, China) using a fluid/property module of TOUGH2 called ECO2N which is adapted from EWASG module [89]. This module was evaluated in a separate study for the CGS process in saline aquifers by Pruess and Spycher [86, 90]. TOUGHREACT, a non-isothermal reactive geochemical transport code, was utilized to simulate the CO₂ disposal in deep aquifers by Xu et al., which was performed by merging the reactive chemistry term into the TOUGH2 framework [91–95]. An efficiency evaluation of CGS was performed in Frio brine pilot project using the TOUGH2 simulator to identify the uncertainties related to nature of the earth by Hovorka et al. [96]. In a previous study at the University of Stuttgart, the MUFTE-UG simulator has been evaluated for CO₂ sequestration in various fields of application such as simulation, CO₂SINK, and CO₂TRAP [97, 98]. At the Ketzin CO₂ storage site, the ECLIPSE 100/300 and MUFTE-UG codes were employed to perform a history matching [99]. Pawar et al. have investigated a preliminary study to model and simulate the CGS in a depleted oil reservoir by ECLIPSE 100 [100]. Another 2/3 dimensional simulation survey with consideration of reactive flow and transport in deep saline aquifers has been performed by Kumar et al. with GEM simulator (computer modeling groups) [101]. ECLIPSE and DuMux simulators are also taken into consideration to understand the thermal effect during CO₂ injection and movement in the porous medium.

According to the CGS simulation methods, there have been some comparative investigations between the various simulators, such as reported by David et al. and Jiang [102]. David et al. have compared six simulators for numerical simulation of CGS in coal beds: (1) GEM, (2) ECLIPSE, (3) COMET2, (4) SIMED II, (5) GCOMP, and (6) METSIM 2. Additional features are needed to be taken into consideration based on Law et al., such as coal matrix swelling, diffusion of mixed gas, non-isothermal effect, water movement, and so on [103]. According to the recent survey by David et al. GEM and SIMED II are suitable to consider multi-component liquids while ECLIPSE and COMET 2 can handle only two component fluids [103, 104]. In 2011, Jiang demonstrated an overview of the various simulator applications and their numerical features including TOUGHREACT, MUFTE, GEM, ECLIPSE, DuMux, COORES, FEHM, ROCKFLOW, SUTRA, and other types of simulators. Numerical methods and physical models play an important role in the simulators outcomes. Selecting the best simulator among those presented above is highly based on the desired application. For example, the ELSA simulator can be applied efficiently in semi-analytical estimation of fluid distributions; ROCKFLOW is

suitable in the case of multi-phase flow and solute transport modeling; GEM is an aqueous geochemistry tool while for the low-temperature situation PHREEQC is more applicable; and for the multi-component, three phase, and 3D fluid flow simulation with consideration of reservoir heterogeneities, COORES would be a robust means [85, 102, 104, 105]. Zhang et al. had a quick look on different types of simulators mentioned earlier and have suggested a new parallel multi-phase fluid flow simulator for CGS in saline aquifers called TOUGH+CO₂ which has been developed on the basis of a modified TOUGH2 family of codes, TOUGH+ and TOUGH2-MP including all the ECO2N features capabilities [83]. This brand new simulator has proved to be a successful and robust means, which has been used in a number of large-scale simulation projects [106–113].

Another group of surveys has focused on the direct modeling of some effective transport phenomena which are essential for predicting parameters that have an important role in underground gas sequestration process such as diffusivity and convection. Azin et al., in 2013, have conducted study regarding correct measurement of diffusivity coefficient [114]. The modeling was based on a method proposed by Sheika et al. to analyze pressure decline data and the impact of pressure and temperature on the measurement of diffusivity coefficient [114]. GholamiY., et al., in 2015, have also investigated the measurement of CO₂ diffusivity in synthetic and saline aquifer solutions at reservoir conditions with emphasis on the role of ion interactions [114–117]. A non-iterative thermodynamic predictive model has investigated by Azin et al. to calculate the effect of gas solubility [118–120]. The effects of convective dissolution and diffusivity mixing have also been surveyed with finite-element method by GholamiY., et al. They have used Streamline Upwind Petrov-Galerkin (SUPG) method and crosswind artificial diffusion and found that the dissolution is controlled by convective dissolution in bulk water [115, 121]. Another numerical simulation was done by Azin et al. to predict the onset of instability in CO₂ underground injection [114]. It was found that depending on Rayleigh number, there is a wave number at which instability occurs earlier and grows faster [114].

4. CGS: Monitoring and Verification

Precise monitoring and verification is required to have an appropriate risk management strategy for the CGS projects [1]. The monitoring and verification process should be commenced from site selection and characterization followed by atmospheric and remote sensing, near and deep surface methods, as well as well bore-monitoring techniques. Different types of monitoring tools are introduced and used in recent literature: acoustic velocity structure imaging by seismic, density distribution imaging by gravity, electrical resistivity structure imaging, and fluid content imaging of potential reservoir rocks by the electromagnetic methods [20, 122]. After injecting the CO₂ into the sequestration sites, electromagnetic and gravitation sensors are employed for seismic surveys of storage integrity such as CO₂ flow and transportation quality in porous media and behavior of cap rock in contact to the CO₂. The leakage measurement in atmospheric level can be done by open path, flux tower, and InSAR systems (satellite-based infrared and interferometric synthetic aperture radar) [20].

Otway Basin Pilot project in Australia is the first CGS project in which monitoring techniques were used [122]. In 2010, the CSEM have considered landing base imaging and passive magnetotelluric in deep crustal scales surveys by Sreitch and colleagues [124]. According to the surveys performed by Arts et al. and Chadwick et al., the 4D gravity and seismic techniques have been successfully accomplished in Sleipner site [125–127]. The 4D vertical seismic profiling (VSP) has been commonly used to quantitative monitoring of the CO₂ plume with tracer injection, well logging, micro-seismic and pressure–temperature measurements which is applied successfully at Frio and Nagaoka project [128–144]. In Frio Brine and Otway Pilot projects, tracer monitoring has been employed to assess the CO₂ breakthrough [145, 146]. The Eddy covariance and hyperspectral imaging in a shallow subsurface site are important computational issues that were examined to monitor the CO₂ leakage in Montana [147, 148]. Another successful surface monitoring technique tested at In Salah project was InSAR which was incorporated into other monitoring techniques such as seismic, gravity, and electromagnetic [149–153]. At Ketzin sequestration site, the monitoring methods included cross-hole resistivity, seismic, and microbiology with temperature and pressure profiling [154–160].

5. Conclusions

In summary, the methods of theoretical and effective capacity estimation of CO₂ storage comprise volumetric and compressibility methods, flow mathematical and simulation models, dimensional analysis, analytical investigation and Japanese/Chinese methodology.

The CSLF model employs a techno-economic resource pyramid in the capacity estimation process for depleted oil and gas reservoir, while the DOE model utilizes volumetric equations and Monte Carlo approach by incorporating various trapping mechanisms. According to the CO₂CRC, storage capacity classification in terms of oil and gas fields is the easiest among the other geological options due to the greater amount of data. A volumetric equation has been proposed to CO₂ storage estimation in the most favorable storage option (saline aquifers) while each type of trapping mechanism is also needed for calculation of the basin-scale assessments. The CSLF methodology has been considered for deep saline aquifers as well as depleted oil and gas reservoir based on structural and stratigraphic trapping mechanisms. Estimation through mineral trapping cannot be applied at the regional and basin scales due to lack of data availability. The only remaining approach, numerical simulation, is suitable for site and local scale for a long period of time. Despite the application of the hydrodynamic trapping mechanism in various time scales, it cannot be evaluated at regional- and basin-scale estimation. To calculate the storage capacity based on compressibility concept, a more comprehensive equation has been addressed recently including flow simulation employing volumetric formulas and more reservoir parameters.

In coal bed capacity estimation, the Langmuir equation provides a simple and efficient relation for single layer low-pressure conditions. In the case of high pressure and high temperature, Bi Langmuir, extended Langmuir, Sips, Langmuir-Freundlich, Toth, UNILAN, two-dimensional

EOS, LRC (loading ratio correlation), Dubinin–Radushkevich (D-R), and Dubinin-Astakhov (D-A) are more suitable.

One of the most efficient means for reservoir modeling is the TOUGH2 simulator developed in Rio Vista reservoir and an extension of EOS7R and EWASG modules also has been proposed to simulate the gas and water flow called EOS7C. A fluid/property module of TOUGH2 called ECO₂N has been utilized for CO₂ modeling in saline aquifers. TOUGHREACT, a non-isothermal reactive geochemical transport code, was utilized to simulate the CO₂ disposal in deep aquifers by entering the reactive chemistry term into the TOUGH2 framework. MUFTE-UG simulator has been evaluated for CO₂ sequestration in various fields of application such as simulation, CO₂SINK, and CO₂TRAP. Another survey with consideration of reactive flow and transport in deep saline aquifers has been performed using the GEM simulator. ECLIPSE and DuMux simulators are also taken into consideration in a study to understand the thermal effect during CO₂ injection and movement in the porous medium.

Six simulators including GEM, ECLIPSE, COMET2, SIMED II, GCOMP, and METSIM2 have been compared for CGS in coalbeds. GEM and SIMED II simulators are suitable for multi-component liquids while ECLIPSE and COMET2 can handle only two component fluids. Other comparison studies including TOUGHREACT, MUFTE, GEM, ECLIPSE, DuMux, COORES, FEHM, ROCKFLOW, SUTRA, and other types of simulators have been carried out throughout the world. Selecting the best simulator among those presented is highly based on the desired application. The ELSA simulator can be applied efficiently in semi-analytical estimation of fluid distributions. ROCKFLOW is suitable in the case of multi-phase flow and solute transport modeling. GEM is an aqueous geochemistry tool, while for the low temperature situation PHREEQC is more applicable. For multi-component, three phase, and 3D fluid flow simulation with consideration of reservoir heterogeneities, COORES would be a robust means. The new parallel multi-phase fluid flow simulator for CGS in saline aquifers called TOUGH+CO₂ has been developed on the basis of a modified TOUGH2 family of codes, TOUGH+ and TOUGH2-MP including all the ECO₂N feature capabilities and has proved to be a successful and robust means in a number of large scale simulation projects.

The CSEM have considered landing base imaging and passive magnetotelluric in deep crustal scale surveys in 2007. The 4D gravity and seismic methods have performed well in the Sleipner project. The 4D vertical seismic profiling (VSP) has been commonly used for quantitative monitoring of the CO₂ plume with tracer injection, well logging, and micro-seismic and pressure-temperature measurements with successful application at Frio and Nagaoka. In Frio Brine and Otway Pilot projects, tracer monitoring has been employed to assess the CO₂ breakthrough. The Eddy covariance and hyperspectral imaging in a shallow subsurface site are important computational issues that were examined to monitor the CO₂ leakage in Montana. Another successful surface monitoring technique tested at In Salah project was InSAR which incorporated to other monitoring techniques such as seismic, gravity, and electromagnetic. At Ketzin sequestration site, the monitoring methods included cross-hole resistivity, seismic, and microbiology with temperature and pressure profiling.

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