

U.S. DOE methodology for the development of geologic storage potential for carbon dioxide at the national and regional scale

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ABSTRACT

A detailed description of the United States Department of Energy (US-DOE) methodology for estimating CO₂ storage potential for oil and gas reservoirs, saline formations, and unmineable coal seams is provided. The oil and gas reservoirs are assessed at the field level, while saline formations and unmineable coal seams are assessed at the basin level. The US-DOE methodology is intended for external users such as the Regional Carbon Sequestration Partnerships (RCSPs), future project developers, and governmental entities to produce high-level CO₂ resource assessments of potential CO₂ storage reservoirs in the United States and Canada at the regional and national scale; however, this methodology is general enough that it could be applied globally. The purpose of the US-DOE CO₂ storage methodology, definitions of storage terms, and a CO₂ storage classification are provided. Methodology for CO₂ storage resource estimate calculation is outlined. The Log Odds Method when applied with Monte Carlo Sampling is presented in detail for estimation of CO₂ storage efficiency needed for CO₂ storage resource estimates at the regional and national scale. CO₂ storage potential reported in the US-DOE's assessment are intended to be distributed online by a geographic information system in NatCarb and made available as hard-copy in the *Carbon Sequestration Atlas of the United States and Canada*. US-DOE's methodology will be continuously refined, incorporating results of the Development Phase projects conducted by the RCSPs from 2008 to 2018. Estimates will be formally updated every two years in subsequent versions of the *Carbon Sequestration Atlas of the United States and Canada*.

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1. Introduction

Estimates of CO₂ storage potential are required to assess the potential for carbon capture and storage (CCS) technologies to contribute towards the reduction of CO₂ emissions. Governments and industries worldwide rely on CO₂ storage potential estimates for broad energy-related government policy and business decisions. Dependable CO₂ storage estimates are necessary to ensure successful deployment of CCS technologies (Bachu et al., 2007; Bradshaw et al., 2007). Several groups worldwide are conducting initiatives for assessing CO₂ geologic storage potential (Bachu

et al., 2007; Bennion and Bachu, 2008; Birkholzer and Zhou, 2009; Birkholzer et al., 2009; Bradshaw et al., 2007; Brennan et al., 2010; Burruss et al., 2009; CEF, 2010; CO2CRC, 2008; CSLF, 2010; DOE-NETL, 2006, 2008, 2010a; Economides and Ehlig-Economides, 2009; Gorecki et al., 2009a,b,c; GSQ, 2010; IEA GHG, 2009; Koide et al., 1992; Kopp et al., 2009a,b; Leetaru et al., 2009; Szulczewski and Juanes, 2009; van der Meer, 1992, 1993, 1995; van der Meer and van Wees, 2006; van der Meer and Egberts, 2008a,b; van der Meer and Yavuz, 2009; Xie and Economides, 2009; Zhou et al., 2008).

This paper provides a detailed description of the United States Department of Energy's (US-DOE's) methodology for estimating CO₂ storage potential. This methodology was developed through US-DOE's Regional Carbon Sequestration Partnerships (RCSPs) initiative (DOE-NETL, 2006, 2008, 2010a). The following discussion includes: the purpose behind the US-DOE CO₂ storage methodol-

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ogy; definitions of storage estimates; a description of CO₂ storage classification; the methodology for CO₂ storage resource estimate calculation; the methodology for calculating CO₂ storage efficiency used in resource estimates; and a critical assessment of CO₂ storage resource calculations.

2. Purpose of the US-DOE CO₂ storage methodology

The US-DOE methodology is intended for external users such as the Regional Carbon Sequestration Partnerships (RCSPs), future project developers, and governmental entities to produce high-level CO₂ resource assessments of potential CO₂ storage reservoirs in the United States and Canada at the regional and national scale, however, the methodology is general enough to be applied globally. The US-DOE's methodology evaluated three types of storage formations – oil/gas reservoirs, saline formations, and unmineable coal seams. The oil/gas reservoirs were assessed at the field level, while saline formations and unmineable coal seams were assessed at the basin level. The CO₂ storage potential reported in US-DOE's assessment is intended to be distributed online by a geographic information system in NatCarb (DOE-NETL, 2010b) and made available as hard-copy in the *Carbon Sequestration Atlas of the United States and Canada* (DOE-NETL, 2006, 2008, 2010a). US-DOE's methodology will be regularly refined, incorporating results of the Development Phase projects conducted by the RCSPs from 2008 to 2018. Estimates will be formally updated every two years in subsequent versions of the *Carbon Sequestration Atlas of the United States and Canada*.

Because the US-DOE methodology is intended to produce high level CO₂ resource estimates of potential geologic storage in the United States and Canada at the regional and national scale, the estimates of CO₂ geologic storage have a high degree of uncertainty. Reasons for this uncertainty include the lack (or sparsity) of wells penetrating potential storage formations and formation heterogeneity, resulting in undefined rock properties. Because of this uncertainty, estimates from the US-DOE methodology are not intended as a substitute for site-specific characterization and assessment. As the site characterization process proceeds at individual CO₂ storage sites, additional site-specific data will likely be collected and analyzed, thereby reducing uncertainty. These data include, but are not limited to, site-specific lithology, porosity, and permeability measurements. Incorporation of these site-specific data allows for the refinement of CO₂ storage resource estimates and development of CO₂ storage capacities by future potential commercial project developers.

3. US-DOE definitions of storage estimates

As discussed in the Introduction, several groups have proposed methods for assessing CO₂ geologic storage potential; however, definitions of storage terms vary according to the organization developing the methodology. The US-DOE methodology is based on volumetric methods for estimating subsurface volumes, *in situ* fluid distributions, and fluid displacement processes (Calhoun, 1982). These methods are widely and routinely applied in petroleum resource, groundwater resource, underground natural gas storage volume, Underground Injection Control (UIC) disposal volume, and CO₂ storage volume estimates (Bachu, 2008; Bachu et al., 2007; Calhoun, 1982; Frailey et al., 2006; Lake, 1989). Subsurface storage volume estimates depend on geologic properties (area, thickness, and porosity of formations) and the efficiency of storage (the fraction of the accessible pore volume that will be occupied by the injected CO₂). Storage efficiency was determined using Monte Carlo sampling, which includes efficiency terms to define the pore volume that is amenable to geologic storage and displacement terms

to define the pore volume immediately surrounding a single CO₂ injector well. This section defines CO₂ storage terms used in the US-DOE methodology.

3.1. CO₂ storage resource estimates

CO₂ storage resource estimates represent the fraction of pore volume in a formation of interest that will be occupied by CO₂ injected through drilled and completed wellbores meeting screening criteria. These criteria include the following, but are not limited to: (1) pressure and temperature conditions; (2) isolation from shallow potable groundwater,¹ other strata, soils, and the atmosphere; and (3) caprock or seal capillary entry pressure (Bachu, 2008).

CO₂ storage resource estimates consider only physical trapping of CO₂. Other trapping mechanisms such as dissolution of CO₂ in brine and subsequent precipitation or mineralization effects are not taken into account when calculating saline formation CO₂ storage resource estimates. At most reservoir temperatures and pressures, the fraction of injected CO₂ that would dissolve in formation brine during the injection process is so small that it can be neglected, given the other large uncertainties in resource estimation. Additionally, the dissolution of injected CO₂ into brine and carbonate mineral formation reactions are complex processes that are dependent on the temperature, pressure, and brine composition within a formation, as well as the effectiveness of the contact between free phase CO₂, the formation brine and, subsequently, the minerals in the formation strata (Bachu et al., 2007). As described in Section 3.3, CO₂ storage resource estimates are based upon the assumption that *in situ* mobile fluids will either be displaced by the injected CO₂ into distant parts of the same formation or neighboring formations, or managed by means of fluid production, treatment, and disposal in accordance with current technical, regulatory, and economic guidelines.

3.2. CO₂ storage capacity estimates

CO₂ storage capacity estimates represent the geologic storage potential when current economic and regulatory considerations are included. For the development of specific commercial-scale geologic storage sites, economic and regulatory constraints must be considered to determine the portion of the CO₂ storage resource estimate that is available under various development scenarios (Bachu, 2008). Under the most favorable economic and regulatory scenarios, 100% of the estimated CO₂ storage resource would be considered CO₂ storage capacity. US-DOE's methodology does not provide CO₂ storage capacity estimates as they require a higher level of analysis than regional and national scale CO₂ storage resource estimates.

Examples of economic considerations involved with CO₂ storage include the following: CO₂ injection rate and pressure; the number of wells drilled into the formation; types of wells (horizontal versus vertical); the number of injection zones completed in each well; operating expenses; management of *in situ* formation fluids (Zhou et al., 2008); injection site proximity to a CO₂ source (Lucier and Zoback, 2008); and combination with enhanced oil recovery (EOR) or enhanced gas recovery (EGR) activities. When determining CO₂ injection rates, an indication of injectivity must be available from an existing well with adequate tests to indicate CO₂ injection rate

¹ Potable waters, for the purposes of this assessment, represent waters protected by the Safe Drinking Water Act (SDWA) which are defined as waters with less than 10,000 parts per million (ppm) total dissolved solids (TDS) (EPA, 2010). Safe Drinking Water Act, Office of Ground Water & Drinking Water, <http://www.epa.gov/safewater/sdwa>.

directly or, at a minimum, *in situ* permeability. Location and spacing of adjacent wells may influence reservoir pressure and the direction of fluid flow. Use of vertical versus horizontal wells may affect the amount of CO₂ that may be stored at a particular site due to the amount of CO₂ injected into specific locations within the reservoir and the efficiency with which the CO₂ will sweep through the reservoir. Increasing the number of viable injection zones within a reservoir may increase the amount of CO₂ that may be stored. Managing *in situ* formation fluids may increase the amount of pore space available for CO₂ storage and lower the pressure build-up resulting from CO₂ injection, although costs of disposal or reinjection may offset potential benefits. Proximity to CO₂ sources will affect surface CO₂ transportation costs. Operating expenses for all of these activities ultimately will dictate the overall cost of operating a CO₂ storage project within a particular storage reservoir.

Examples of regulatory considerations include the following: protection of potable water; well spacing requirements; maximum injection rates; prescribed completion methods (cased vs. open-hole); proximity to existing wells; treatment of *in situ* fluids and surface usage considerations (Wilson et al., 2003). Many of these considerations are addressed through the Environmental Protection Agency (EPA) Underground Injection Control (UIC) Program's Class VI well proposed rule, which defines specific requirements for CO₂ injection projects. Additional regulatory considerations may exist at the State and Provincial levels. Due to the varied nature of regulatory regimes for potential CO₂ storage reservoirs, CO₂ storage capacity estimates require site-specific assessments.

3.3. Boundary conditions

Defining boundary conditions is necessary for any type of subsurface assessment. Two end member systems, open and closed, can be used to define the boundaries for potential CO₂ storage reservoirs. Open systems are permeable fluid-filled reservoirs where *in situ* fluids will either be displaced away from the injection location into other parts of the formation and/or into neighboring formations (Birkholzer and Zhou, 2009; Gorecki et al., 2009b; IEA GHG, 2009; Nicot, 2008; Zhou et al., 2008). Subsequently, the primary constraints on the percentage of pore space that can be filled with CO₂ in open systems are due to displacement efficiencies, rather than pressure increases, although there will often be a need to define a maximum bottom-hole injection pressure to reduce risks associated with injection (Gorecki et al., 2009b; IEA GHG, 2009; Zhou et al., 2008). Displacement of fluids from reservoirs has been examined in recent studies, which focus on potential effects of fluid migration to other subsurface geological formations (Birkholzer and Zhou, 2009; Birkholzer et al., 2009; Leetaru et al., 2009; Nicot, 2008; Zhou et al., 2008).

Closed systems are fluid-filled reservoirs where *in situ* fluid movement is restricted within the formation by means of impermeable barriers (Birkholzer and Zhou, 2009; Gorecki et al., 2009b; IEA GHG, 2009; Nicot, 2008; Zhou et al., 2008). Storage volume in closed systems is then constrained by the compressibility of the formation's native fluid and rock matrix (van der Meer, 1992, 1993, 1995; van der Meer and Egberts, 2008a,b; van der Meer and Yavuz, 2009). In addition, the CO₂ injection pressure cannot exceed the maximum allowable pressure of the formation, as over-pressurization may damage natural formation seals (Burruss et al., 2009; Gorecki et al., 2009b; Zhou et al., 2008). The very low compressibility of formation fluids and rocks limit the capacity of closed systems to a very small percentage of total pore volume (Gorecki et al., 2009b; Xie and Economides, 2009; Zhou et al., 2008). Even in a fault-compartmentalized closed system that has shale confining units above and below, the small permeability of the shale may allow for pressure bleed-off which helps to reduce pressure and increases capacity beyond the compressibility esti-

mates (Birkholzer and Zhou, 2009; Birkholzer et al., 2009). Further, closed systems can respond like open systems by means of managing, treating, and disposing of *in situ* fluids in accordance with current technical, regulatory, and economic guidelines (Birkholzer and Zhou, 2009; Gorecki et al., 2009b; IEA GHG, 2009; Nicot, 2008; Zhou et al., 2008).

As defined in Section 3.1, storage resource estimates are based on open systems in which *in situ* fluids will either be displaced from the injection zone or managed. Accordingly, CO₂ storage resource estimates provide an upper boundary for CO₂ storage. Realization of the full CO₂ storage resource estimate as a capacity estimate will rely on how site-specific geology, economics, and regulations restrict management of *in situ* fluids.

4. CO₂ storage classification

The process of identifying suitable geologic storage sites involves a methodical and careful analysis of the technical and non-technical features of a potential site. This process is analogous to the methods used in the petroleum industry to mature a project through a classification of resource classes and project status subclasses until the project begins producing hydrocarbons. Recent CO₂ storage classifications systems have been proposed (Bachu et al., 2007; Bradshaw et al., 2007; Burruss et al., 2009; Gorecki et al., 2009b; IEA GHG, 2009). It is envisioned that a CO₂ Geologic Storage Classification System would follow the same processes developed by the petroleum industry in a bottom up progression based on analyses conducted to reduce the project development risk. The proposed framework would contain three distinct phases of evaluation (Exploration Phase, Site Characterization Phase, and Implementation Phase) corresponding to each resource class and further subdivided into project sub-classes (Table 1) (DOE-NETL, 2010c).

The Exploration Phase evaluates resources classified as Prospective Storage Resources and is divided into three project sub-classes (Potential Sub-Regions, Selected Areas, and Qualified Sites). Each project sub-class undergoes an evaluation process (Site Screening, Site Selection, and Initial Characterization) that builds on previous analyses to pare down larger Sub-Regions into Qualified Site(s). The three evaluation processes are discussed in more detail below:

- Site Screening involves analysis of three components (regional geologic data, regional site data, and social data) to develop and rank a list of Selected Areas within a Potential Sub-Region to elevate to the Site Selection evaluation. The analysis conducted highlights the most promising Selected Areas for geologic storage, while eliminating those that do not meet a developer's criteria.
- Site Selection involves analyzing the most promising Selected Areas in more detail, to ensure only those that meet critical technical and economic criteria advance for further evaluation. Analysis is conducted on five separate components, including subsurface geologic data, regulatory requirements, model data, site data, and social data. At the completion of this stage, the developer will have a list of potential Qualified Site(s) that can be assessed during the final evaluation stage.
- Initial Characterization involves analysis on one or more of the higher ranked Qualified Site(s). Several components are analyzed, including baseline data, regulatory requirements, model data, social data, and a site development plan. These results should provide enough information to qualify discovered storage at the Qualified Site(s) as Contingent Storage Resource.

At the completion of the Exploration Phase, a Qualified Site moves into the Site Characterization Phase, classifying the storage as Contingent Storage Resources with three project sub-classes:

Table 1
CO₂ geologic storage classification system.

Petroleum Industry		CO ₂ Geological Storage	
Reserves		Implementation	Capacity
On Production	Active Injection		
Approved for Development	Approved for Development		
Justified for Development	Justified for Development		
Contingent Resources		Site Characterization	Contingent Storage Resources
Development Pending	Development Pending		
Development Unclassified or On Hold	Development Unclassified or On Hold		
Development Not Viable	Development Not Viable		
Prospective Resources		Exploration	Prospective Storage Resources
Prospect	Qualified Site(s)		
Lead	Selected Areas		
Play	Potential Sub-Regions		

Prospective Storage Resources	
Exploration	Project Sub-class
	Qualified Site(s)
	Selected Areas
	Potential Sub-Regions
	Evaluation Process
	Initial Characterization
	Site Selection
	Site Screening

Development Not Viable, Development Unclassified or on Hold, or Development Pending. Once the appraised Qualified Site is considered commercial, the project would move into the Implementation Phase. The project would first be classified as Justified for Development. Once all necessary approvals and permits have been obtained and capital funds committed, the project elevates to Approved for Development, which would give way to Active Injection. The successful characterization of a site is one of the most important steps in ensuring the safe and economic operation of a geologic CO₂ storage site.

5. US-DOE methodology for CO₂ storage resource estimate calculation

Environments considered for CO₂ storage were categorized into five major geologic systems: oil and gas reservoirs, saline formations, unmineable coal areas, shale, and basalt formations. Where possible, CO₂ storage resource estimates have been quantified for oil and gas reservoirs, saline formations, and unmineable coal areas, whereas shale and basalt formations are presented as future opportunities and not assessed in the current US-DOE methodology. Methods available for estimating subsurface volumes are widely and routinely applied in hydrocarbon, ground water, underground natural gas storage, and Underground Injection Control (UIC) disposal-related estimations (Calhoun, 1982; Frailey et al., 2006; Lake, 1989). Two different approaches are typically used to estimate subsurface injection volumes; they are defined as static and dynamic methods (Calhoun, 1982). Static methods used to estimate CO₂ storage potential are based on volumetric and

compressibility-based models (Bachu, 2008; Bachu et al., 2007; Bradshaw et al., 2007; Burruss et al., 2009; Gorecki et al., 2009b; IEA GHG, 2009; Kopp et al., 2009a,b; Szulczewski and Juanes, 2009; van der Meer, 1995; van der Meer and Egberts, 2008a,b; van der Meer and Yavuz, 2009). Volumetric methods are applied when it is generally assumed that the formation is open and that formation fluids are displaced from the formation or managed via production. If it is demonstrated that the system is closed, volumetrics of the storage system would still be calculated, but the resource estimate would be based on how much of that space could be compressed due to the injection of CO₂. Meaningful dynamic simulations typically cannot be done before site-specific data are collected from the field of interest, such as field-measured injection rates and/or well testing. The US-DOE methodology uses the volumetric approach for estimating CO₂ storage resource potential in oil and gas reservoirs, saline formations, and unmineable coal seams.

For the US-DOE methodology, CO₂ storage resource estimates for oil/gas reservoirs are reported at the field level, whereas saline formations and unmineable coal seams are reported at the basin level. The field level is a well-defined spatial scale on a technical and regulatory basis, and captures complexities inherent to specific fields such as leases and wells. In addition, field level analysis facilitates data manipulation, storage, and access. The field level can be summed to provide estimates at state, basin, or regional scales. It is also possible to cross-check storage estimates against readily available state, province, and national production numbers such as the Energy Information Administration [EIA] and state or provincial oil and gas commissions. The basin level for saline formations and unmineable coal seams are defined at natural geologic boundaries. Where basins straddle more than one region, one RCSP assumed primary responsibility for the basin, while the other RCSP provided the needed data in its portion of the basin. Determination of state CO₂ storage resource estimations where basins straddle more than one state was made by dividing the total CO₂ storage resource estimate for the basin into 10 × 10 kilometer grids and summing the total for the state. Where available, data provided with a measured 10 × 10 kilometer grid resolution are reported directly. Because oil and gas reservoirs are reported at the field scale and saline formations and unmineable coal seams are reported at the basin level, cross comparison of estimates may not be useful.

5.1. Oil and gas reservoir CO₂ storage resource estimating

By their very existence, hydrocarbon reservoirs demonstrate the capability to store significant quantities of buoyant fluids. Typical petroleum systems consist of an interval of permeable reservoir rock, overlaid by an impermeable unit called a caprock or seal. Additionally a geometric component formed either by the depositional system or later tectonic alteration of the rock is necessary and is called a trap. Thus, oil and gas fields are excellent targets for CO₂ geologic storage, as the geologic conditions that trap oil and gas are also generally conducive to long-term CO₂ storage.

The US-DOE methodology defines CO₂ storage resource estimates on a volumetric basis for oil or gas reservoirs that have hosted natural accumulations of oil or gas and that could be used to store CO₂ in the future. No distinction is made in this assessment for the maturity of the field. Because oil and gas fields can be productive across a wide variety of depths, no minimum or maximum depth criteria were used for CO₂ storage resource estimates. Oil and gas fields with a water total dissolved solids (TDS) concentration of 10,000 ppm (EPA, 2010) and higher were included (to maintain consistency with saline and coal formation TDS cutoffs), unless specifically noted and justified. For example, the water quality in oil and gas fields may be classified as non-potable due to oil and gas contamination.

Storage volume methodology for oil and gas fields was based on quantifying the volume of oil and gas that has or could be produced, and assuming that it could be replaced by an equivalent volume of CO₂. However, there is not always a one-to-one relationship between oil and gas volume footprint and a trap footprint for holding hydrocarbons (Nicot and Hovorka, 2009). Both oil/gas and CO₂ volumes are calculated at initial formation pressure or a pressure that is considered a maximum CO₂ storage pressure. Two main methods, described below, were used to estimate the CO₂ storage volume: (1) a volumetric-based CO₂ storage resource estimate and (2) a production-based CO₂ storage resource estimate. The method used by each RSCP was based on available data. The two methods have storage efficiency factors built into their respective equations and, therefore, CO₂ storage resource estimates are proposed as a single value for oil and gas fields. Production-based CO₂ storage resource estimates are generally preferred over volumetric-based CO₂ storage resource estimates because production data contain detailed information collected from the formation. If no production data are available, then volumetric-based CO₂ storage resource estimates may be applied. In the oil and gas industry, hydrocarbon recovery related attributes are calculated and applied with respect to the original oil or gas in place (at surface conditions, e.g. stock tank barrels of oil) regardless of the maturity of the oil or gas field development. Likewise, for estimating CO₂ storage resource in oil and gas reservoirs, CO₂ storage efficiency was developed as a function of the original hydrocarbon in place.

The volumetric-based CO₂ storage resource estimate is based on the standard industry method to calculate original oil-in-place (OOIP) or original gas-in-place (OGIP) (Calhoun, 1982; Lake, 1989). The general form of the volumetric equation to calculate the CO₂ storage resource mass estimate (G_{CO_2}) for geologic storage in oil and gas reservoirs is as follows:

$$G_{CO_2} = Ah_n\phi_e(1 - S_{wi})B\rho_{CO_2std}E_{oil/gas} \quad (1)$$

The product of the area (A), net thickness (h_n), average effective porosity (ϕ_e), original hydrocarbon saturation ($1 - \text{initial water saturation}$, expressed as a fraction [S_{wi}]), and the initial oil (or gas) formation volume factor (B) yield the OOIP (or OGIP). The standard CO₂ density (ρ_{CO_2std}) converts standard CO₂ volume to mass. The storage efficiency factor ($E_{oil/gas}$) is derived from local CO₂ EOR experience or reservoir simulation as standard volume of CO₂ per volume of OOIP. In oilfield terms, the CO₂ EOR oil recovery factor and the CO₂ net utilization are equal to the storage efficiency factor. Because of previous extensive experience in estimating volumetrics of oil and gas formations; regional, play, or formation-specific efficiency values are used for CO₂ storage estimating. Table 2 summarizes the terms shown in Eq. (1).

A production-based CO₂ storage resource estimate is possible if acceptable records are available on volumes of oil and gas produced. Produced water is not considered in the estimates, nor is injected water (waterflooding), although these volumes may be useful in site-specific calculations (Bachu et al., 2007). In cases where a field has not reached a mature stage, it is beneficial to apply decline curve analysis to better approximate the estimated ultimate recovery (EUR), which represents the expected volume of produced oil and gas (Calhoun, 1982; Lake, 1989).

It is necessary to apply an appropriate reservoir volume factor (B) to convert surface oil and gas volumes (reported as production) to subsurface volumes (including correction of solution gas volumes if gas production in an oil reservoir is included). No area, column height, porosity, residual water saturation, or estimation of the fraction of OOIP that is accessible to CO₂ is required because production reflects these reservoir characteristics. If information is available, it is possible to apply efficiency to production data to convert them to CO₂ storage volumes; otherwise replacement

Table 2
Oil and gas reservoir CO₂ storage resource estimating.

Parameter	Units ^a	Description
G_{CO_2}	M	Mass estimate of oil and gas reservoir CO ₂ storage resource.
A	L ²	Area that defines the oil or gas reservoir that is being assessed for CO ₂ storage.
h_n	L	Net oil and gas column height in the reservoir.
ϕ_e	L ³ /L ³	Average effective porosity in volume defined by the net thickness.
S_{wi}	L ³ /L ³	Average initial water saturation within the total area (A) and net thickness (h_n).
B	L ³ /L ³	Fluid formation volume factor; converts standard oil or gas volume to subsurface volume (at reservoir pressure and temperature), e.g. stock tank volume of oil per reservoir volume of oil.
ρ_{CO_2std}	M/L ³	Standard density of CO ₂ evaluated at standard pressure and temperature.
$E_{oil/gas}$	L ³ /L ³	CO ₂ storage efficiency factor, the volume of CO ₂ stored in and oil or gas reservoir per unit volume of original oil or gas in place (OOIP or OGIP).

^a L is length; M is mass.

of produced oil and gas by CO₂ on a volume-for-volume basis (at reservoir pressure and temperature) may be acceptable.

5.2. Saline formation CO₂ storage resource estimating

Saline formations are composed of water-saturated porous rock and capped by one or more regionally extensive low-permeability rock formations. A saline formation assessed for CO₂ storage is defined as a porous and permeable body of rock containing water with TDS greater than 10,000 ppm (EPA, 2010). A saline formation can include more than one named geologic stratigraphic unit or be defined as only a part of a stratigraphic unit. Mechanisms for CO₂ storage in saline formations include structural trapping, hydrodynamic trapping, residual trapping, dissolution, and mineralization (Bachu et al., 2007; Kopp et al., 2009b; Xie and Economides, 2009). Structural and hydrodynamic trapping are initially the dominant trapping mechanisms and are the focus of the US-DOE methodology.

Saline formations assessed for storage are restricted to those meeting the following basic criteria: (1) pressure and temperature conditions in the saline formation are adequate to keep the CO₂ liquid or supercritical; (2) a suitable seal system, such as a caprock, is present to limit vertical flow of the CO₂ to the surface; and (3) a combination of hydrogeologic conditions isolates the CO₂ within the saline formation. These criteria also apply to existing UIC and other regulations and are relevant to capacity assessment as well, but the criteria are first incorporated into CO₂ storage resource assessments.

The storage of CO₂ in saline formations is limited to sedimentary basins with vertical flow barriers and depths exceeding 800 m. Sedimentary basins include porous and permeable sandstone and carbonate rocks. The 800 m cut-off represents a general attempt to select a depth with pressures and temperatures yielding high density liquid or supercritical CO₂, recognizing that this depth can vary significantly from one location to another. All sedimentary rocks included in the saline formation CO₂ storage resource estimate must have seal systems consisting of low permeability sealing rocks, such as shales, anhydrites, and other evaporates, however, the thickness of these sealing systems is not considered in this methodology. For increasing confidence in storage resource estimates, other criteria including seal effectiveness (e.g., salinity and pressure above and below the seal system), minimum permeability, minimum threshold capillary pressure,

Table 3
Saline formation CO₂ storage resource estimating.

Parameter	Units ^a	Description
G_{CO_2}	M	Mass estimate of saline formation CO ₂ storage resource.
A_t	L ²	Geographical area that defines the basin or region being assessed for CO ₂ storage.
h_g	L	Gross thickness of saline formations for which CO ₂ storage is assessed within the basin or region defined by A .
ϕ_{tot}	L ³ /L ³	Total porosity in volume defined by the net thickness.
ρ	M/L ³	Density of CO ₂ evaluated at pressure and temperature that represents storage conditions anticipated for a specific geologic unit averaged over h_g and A_t .
E_{saline}	L ³ /L ³	CO ₂ storage efficiency factor that reflects a fraction of the total pore volume that is filled by CO ₂ .

^a L is length; M is mass.

and fracture propagation pressure of a seal system should be considered.

The volumetric equation to calculate the CO₂ storage resource mass estimate (G_{CO_2}) for geologic storage in saline formations is:

$$G_{CO_2} = A_t h_g \phi_{tot} \rho E_{saline} \quad (2)$$

The total area (A_t), gross formation thickness (h_g), and total porosity (ϕ_{tot}) terms account for the total bulk volume of pore space available. The CO₂ density (ρ) converts the reservoir volume of CO₂ to mass. Rather than using an irreducible water saturation parameter explicitly, the storage efficiency factor (E_{saline}) reflects the fraction of the total pore volume that will be occupied by the injected CO₂. As described in Section 6.1, E_{saline} factors range between 0.40 and 5.5 percent over the 10th to 90th percent probability range. Table 3 summarizes the terms shown in Eq. (2).

5.3. Unmineable coal seam CO₂ storage resource estimating

CO₂ storage within coal seams normally involves displacement of coalbed methane (CBM). Initial CBM recovery methods, such as dewatering and depressurization, leave a portion of methane (CH₄) in the formation. CO₂ sequestration in unmineable coal seams may provide the added benefit of enhanced coalbed methane (ECBM) recovery, which is controlled by the relative affinity of the two gases to the sorption sites, their relative mobility, and sorption–desorption kinetics (Li et al., 2010).

Only coal seams containing water with TDS greater than 10,000 ppm merited evaluation for potential CO₂ storage (EPA, 2010). Where the water quality data are scarce or unavailable, analogy to other geological basins was used to estimate the minimum depth criteria. The maximum depth was arbitrarily selected for each basin to account for practicalities of CO₂ storage by sorption in coal. Depending on geothermal and geo-pressure gradients in a formation, gaseous CO₂ adsorption may only be possible down to depths of about 3000 ft (900 m) (Ryan and Littke, 2005). At greater depths and depending on coal rank, supercritical CO₂ may enter the solid coal and change its properties, which results in swelling of the coal matrix and causes injectivity problems (Metz et al., 2005). Cleat closure induced by increasing effective stress will further decrease permeability to such extent that coalbed methane cannot be produced below 5000 ft (1500 m) (Bachu et al., 2007). Currently, this is defined as the maximum depth limit for potential CO₂ storage in coal (Metz et al., 2005). Beyond this limit, CO₂ storage is limited by the compression costs, escalating below 11,000 ft (3300 m) (van der Meer, 1993).

Table 4
Unmineable coal seam CO₂ storage resource estimating.

Parameter	Units ^a	Description
G_{CO_2}	M	Mass estimate of CO ₂ resource of one or more coal beds.
A	L ²	Geographical area that outlines the coal basin or region for CO ₂ storage calculation.
h_g	L	Gross thickness of coal seam(s) for which CO ₂ storage is assessed within the basin or region defined by A .
$C_{s,max}$	L ³ /L ³	Adsorbed maximum standard CO ₂ volume per unit of <i>in situ</i> coal volume (Langmuir or alternative); assumes 100% CO ₂ saturated coal conditions; if on dry-ash-free (daf) basis, conversion should be made.
$\rho_{CO_2, std}$	M/L ³	Standard density of CO ₂ .
E_{coal}	L ³ /L ³	CO ₂ storage efficiency factor that reflects a fraction of the total coal bulk volume that is contacted by CO ₂ .

^a L is length; M is mass.

Within the depth intervals selected for a particular basin, a determination was made as to which coals are unmineable by today's state-of-the-art standards of technology. Although advancements in mining technology and changes in the value of the commodity may enable some of the coal seams deemed unmineable today to be mineable in the future, it is beyond the scope of this effort to forecast the long-term developments and their impact. Only coals deemed unmineable are included in this CO₂ storage resource estimate.

The following is the volumetric equation to calculate the CO₂ storage resource mass estimate (G_{CO_2}) for geologic storage in unmineable coal seams:

$$G_{CO_2} = A h_g C_{s,max} \rho_{CO_2, std} E_{coal} \quad (3)$$

The total area (A) and gross area thickness (h_g) terms account for the total bulk volume containing the coal(s) to be assessed. $C_{s,max}$ is the maximum volume of CO₂ at standard conditions that can be sorbed per volume of coal (e.g., the Langmuir isotherm volume constant), and is assumed to be on an *in situ* or “as is” basis. A conversion from mass or dry-ash-free volume basis may be necessary. A component within the calculation of E_{coal} , includes the degree of saturation achievable for an *in situ* coal compared with the theoretical maximum predicted by the CO₂ Langmuir isotherm (Section 6.2). The CO₂ density ($\rho_{CO_2, std}$) converts the standard CO₂ volume in the Langmuir term (C) to mass. The storage efficiency factor (E_{coal}) reflects the fraction of the total bulk coal volume that will store the injected CO₂. As described in Section 6.2, E_{coal} factors range between 21 and 48 percent at the 10th to 90th percent probability range. Table 4 summarizes the terms shown in Eq. (3).

The maximum CO₂ sorption capacity of coal at saturation ($C_{s,max}$), which depends on the coal characteristics and, to a certain extent, on temperature, can be reported on per unit-of-coal-mass basis ($n_{s,max}$). Conversion into per unit-volume basis ($C_{s,max}$) requires the knowledge of coal bulk density ($\rho_{c,dry}$) as well as moisture and/or ash content, depending on the reporting format (such as dry, ash free). The average density of sorbed CO₂ in coal under saturated conditions is described by Eq. (4):

$$C_{s,max} = n_{s,max} \rho_{c,dry} (1 - f_{a,dry}) \quad (4)$$

where $f_{a,dry}$ is the ash weight fraction of the dry coal bulk density ($\rho_{c,dry}$). For consistency with the distinction between the micropore sorption and the hydrodynamic trapping due to fracture porosity, the coal bulk density should be measured as inclusive of micropore volume (e.g., mercury density of coal) (Gan et al., 1972). However, the helium density of coal, which is the most readily available

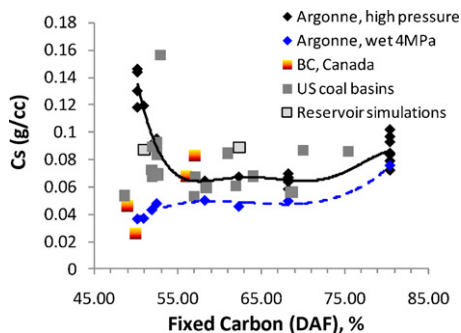


Fig. 1. Average CO₂ Sorption (expressed in g/cm³) vs. Coal Rank (expressed as percent fixed carbon on a dry and ash free basis (daf)). Red and gray solid squares represent experimental data for Canadian and North American coals, respectively. Black and blue solid diamonds represent experimental data for Argonne premium coals at saturation (high pressure) and at low pressure (4 MPa wet), respectively. Gray solid squares with black outline represent data for two reservoir simulations (Botnen et al., 2009; Bromhal et al., 2005; Busch et al., 2003; Chikatamarla et al., 2004; Clarkson and Bustin, 1999; Day et al., 2008a; Durucan and Shi, 2009; Fitzgerald et al., 2005, 2006; Goodman et al., 2007; Harpalani and Mitra, 2010; Harpalani et al., 2006; Jessen et al., 2008; Ozdemir and Schroeder, 2009; Pini et al., 2010; Reeves et al., 2005; Romanov and Soong, 2008; Ross et al., 2009; Siemons and Busch, 2007). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of the article.)

data, is a good approximation as long as the micropore volume is accounted for in the fracture porosity (Huang et al., 1995).

The CO₂ that is stored per unit of coal under reservoir conditions, as opposed to under ideal (maximum) pressure conditions, depends on reservoir pressure after injection, moisture content, and the amount of gas in place (Clarkson and Bustin, 2000). However, the pressure effect can be approximated by a standard (e.g., Langmuir) isotherm equation. For lower rank coals, care should be taken to perform laboratory testing under reservoir conditions because chemical heterogeneity increases the difference in accessible micropore volumes between wet and dry coals observed at low pressure (low surface coverage) (Prinz and Littke, 2005). If data are available, different isotherms for different coal ranks are used. If no CO₂ isotherm is available, isotherms from similar rank coals in analog basins can be used, such as the isotherm data plotted in Fig. 1 (Botnen et al., 2009; Bromhal et al., 2005; Busch et al., 2003; Chikatamarla et al., 2004; Clarkson and Bustin, 1999; Day et al., 2008a; Durucan and Shi, 2009; Fitzgerald et al., 2005, 2006; Goodman et al., 2007; Harpalani and Mitra, 2010; Harpalani et al., 2006; Jessen et al., 2008; Ozdemir and Schroeder, 2009; Pini et al., 2010; Reeves et al., 2005; Romanov and Soong, 2008; Ross et al., 2009; Siemons and Busch, 2007).

6. CO₂ storage efficiency for resource estimates

Carbon dioxide storage efficiency gauges the fraction of the accessible pore volume that will be occupied by the injected CO₂. In open systems, the fraction of accessible pore volume is estimated by the use of geologic terms: area, thickness, and porosity, and displacement terms: areal, vertical, gravity, and microscopic displacement (Lake, 1989). In closed systems, the fraction of accessible pore volume is estimated by compressibility of the formation, compressibility of the *in situ* fluid, the degree of impermeability of the boundaries, and the maximum allowable pressure. As discussed in Section 3, the US-DOE methodology bases efficiency factors calculated for CO₂ storage resource estimates on open systems. Monte Carlo sampling techniques, as described in Sections 6.1 and 6.2, were used to estimate efficiency factors for CO₂ storage resource estimates for both saline formations and unmineable coal seams over the P_{10} , P_{50} , and P_{90} percent probability range. Efficiency in

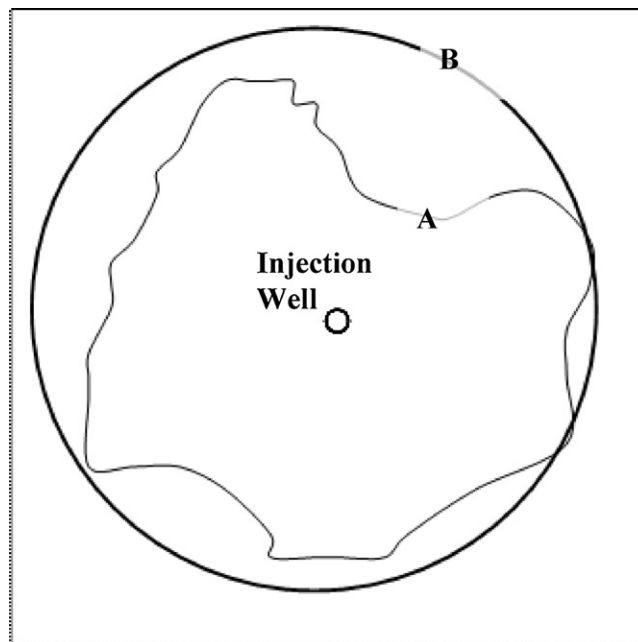


Fig. 2. Top-view of injection well and plume area. The area within the irregular shape inside the circle is the areal view of the 3-dimensional CO₂ plume (A). The area inside the larger circle (B) is the accessible pore volume for areal displacement. The areal displacement term, $E_A = \text{net area contacted by CO}_2 \text{ (A) / Total area (B)}$.

the US-DOE methodology is comprised of statistical properties of geologic and displacement parameters.

6.1. Storage efficiency of saline formations

As described in Section 5.2, overall CO₂ storage resource estimates for saline formations are calculated by Eq. (2).

$$G_{\text{CO}_2} = A_t h_g \phi_{\text{tot}} \rho E_{\text{saline}}$$

For saline formations, the CO₂ storage efficiency factor is a function of geologic parameters such as area (E_{A_n/A_t}), gross thickness (E_{h_n/h_g}), and total porosity ($E_{\phi_e/\phi_{\text{tot}}}$) which reflect the percentage of volume that is amenable to CO₂ sequestration and displacement efficiency components such as areal (E_A), vertical (E_L), gravity (E_g), and microscopic (E_d) which reflect different physical barriers that inhibit CO₂ from contacting 100 percent of the pore volume of a given basin or region (Bachu et al., 2007; Doughty and Pruess, 2004; Koide et al., 1992; Shafeen et al., 2004; van der Meer, 1992). Eq. (5) describes the individual parameters required to estimate the CO₂ storage efficiency factor for saline formations:

$$E_{\text{saline}} = E_{A_n/A_t} E_{h_n/h_g} E_{\phi_e/\phi_{\text{tot}}} E_A E_L E_g E_d \quad (5)$$

The net-to-total area E_{A_n/A_t} ratio is the fraction of the total basin or region area that is suitable for CO₂ storage. The net-to-gross thickness E_{h_n/h_g} ratio is the fraction of the total geologic unit that meets minimum porosity and permeability requirements for injection. The effective-to-total porosity $E_{\phi_e/\phi_{\text{tot}}}$ ratio is the fraction of total interconnected porosity (Table 5).

The displacement terms are described below and shown schematically in Figs. 2 and 3. The areal displacement (E_A) efficiency is the fraction of planar area surrounding the injection well that CO₂ can contact. This term is influenced by areal geologic heterogeneity, such as faults or permeability, and by CO₂ mobility (Lake, 1989). The vertical (geologic layering) displacement (E_L) efficiency is the fraction of vertical cross section or thickness with the volume defined by the area (A) that can be contacted by the CO₂ plume from a single well, which can be affected by the aquifer dip and by

Table 5
Parameters for saline formation efficiency.

Term	Symbol	P_{10}/P_{90} values by lithology			Description
		Clastics	Dolomite	Limestone	
Geologic terms used to define the entire basin or region pore volume					
Net-to-Total Area	$E_{An/At}$	0.2/0.8	0.2/0.8	0.2/0.8	Fraction of total basin or region area with a suitable formation.
Net-to-Gross Thickness	$E_{hn/hg}$	0.21/0.76 ^a	0.17/0.68 ^a	0.13/0.62 ^a	Fraction of total geologic unit that meets minimum porosity and permeability requirements for injection.
Effective-to-Total Porosity	$E_{\phi_e/\phi_{tot}}$	0.64/0.77 ^a	0.53/0.71 ^a	0.64/0.75 ^a	Fraction of total porosity that is effective, i.e., interconnected.
Displacement terms used to define the pore volume immediately surrounding a single well CO ₂ injector.					
Volumetric displacement efficiency	E_V	0.16/0.39 ^a	0.26/0.43 ^a	0.33/0.57 ^a	Combined fraction of immediate volume surrounding an injection well that can be contacted by CO ₂ and fraction of net thickness that is contacted by CO ₂ as a consequence of the density difference between CO ₂ and <i>in situ</i> water.
Microscopic displacement efficiency	E_d	0.35/0.76 ^a	0.57/0.64 ^a	0.27/0.42 ^a	Fraction of pore space unavailable due to immobile <i>in situ</i> fluids.

^a Values from IEA GHG (2009).

CO₂ buoyancy (Lake, 1989). This term is influenced by variations in porosity and permeability between sub-layers in the same geologic unit. If one zone has higher permeability than other zones, the CO₂ will fill this zone quickly and leave the other zones with less or no CO₂. The gravity displacement (E_g) efficiency is the fraction of net thickness that is contacted by CO₂ as a consequence of the density and mobility difference between CO₂ and *in situ* water. In other words, $1 - E_g$ is the portion of the net thickness not contacted by CO₂ because the CO₂ rises within the geologic unit. The microscopic displacement (E_d) efficiency is the fraction of the CO₂ contacted, water-filled pore volume that can be replaced by CO₂ (Lake, 1989). This term is directly related to irreducible water saturation in the presence of CO₂. For the areal, vertical, and gravity

displacement terms, it is assumed that all *in situ* fluids are fully displaced by CO₂. Since 100% displacement of fluid is not theoretically or technically feasible, the microscopic displacement term identifies the fraction of pore space unavailable due to immobile *in situ* fluids (Figs. 2 and 3).

Efficiency estimates using Monte Carlo sampling are based on statistical properties – such as mean values, standard deviation, ranges, and distributions – that describe geologic and displacement parameters. Little information is known regarding the statistical characteristics of saline formations because geologic parameters and formations are not well characterized (Bachu et al., 2007; Burruss et al., 2009; DOE-NETL, 2006, 2008, 2010a; Doughty and Pruess, 2004; Gorecki et al., 2009a,b,c; IEA GHG, 2009). Recently, the International Energy Agency Greenhouse Gas R&D Programme (IEA GHG) (2009) and Kopp et al. (2009a,b) used field data from oil and gas reservoirs and numerical simulations using relative-permeability data for CO₂-brine systems measured in the laboratory (Bennion and Bachu, 2008) to predict appropriate ranges for geologic and displacement parameters for saline formations as a function of lithology. Similar work that predicts parameters for saline formations is also available (Gorecki et al., 2009a,b,c). It was assumed that saline formations do not differ fundamentally from oil and gas reservoirs (IEA GHG, 2009; Kopp et al., 2009a). Table 5 includes values reported by IEA GHG (2009) of the P_{10} and P_{90} ranges of geologic and displacement parameters for clastics, dolomite, and limestone lithologies for saline formations.² The P_{10} notation reflects that there is a 10% probability that the value is less than the P_{10} value and the P_{90} notation reflects that there is a 90% probability that the value is less than the P_{90} value. Because of the difficulty in separating the E_A , E_L , and E_g displacement terms shown in Eq. (5) in a heterogeneous scenario, these terms were combined by IEA GHG (2009) into a single volumetric displacement term, E_V .

In the US-DOE methodology, efficiency, as estimated by Monte Carlo sampling, for saline formations was based directly on the P_{10} and P_{90} ranges for net-to-gross thickness $E_{hn/hg}$, effective-to-total porosity $E_{\phi_e/\phi_{tot}}$, volumetric displacement (E_V), and microscopic displacement (E_d) as reported by IEA GHG (2009) (Table 5). Because no documented data for the area $E_{An/At}$ term are available, it was assumed that CO₂ will occupy between 20 and 80 percent of the formation for the purposes of these simulations (DOE-NETL,

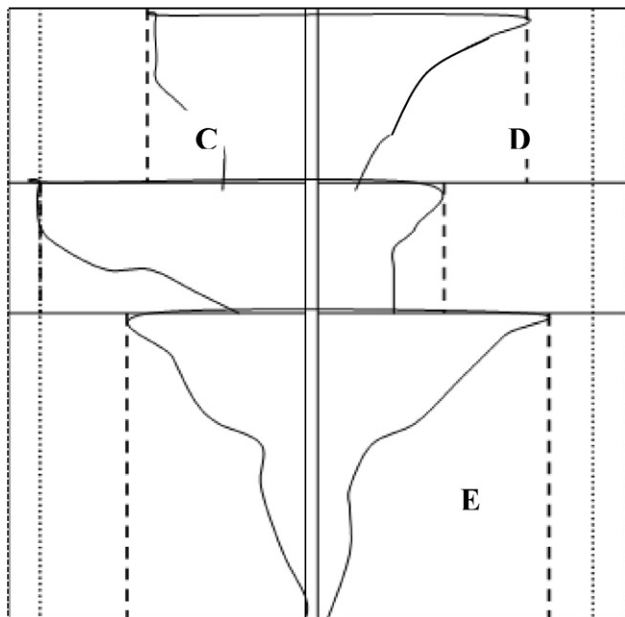


Fig. 3. Side view of injection well and plume area. The outer vertical dotted lines are defined by the outer areal circle (Depicted by B in Fig. 2). The “plume” area enclosed within each interval that is bound by vertical dashed lines represents the numerator of the E_d term (area enclosed within C); the denominator is the entire space outlined by the dotted line (area enclosed within D). Within the area bound by the dashed lines, the lower portion is not contacted due to gravity (area depicted by E) and is removed by the E_g term. The E_d term then defines the CO₂ displacement efficiency in the plume region.

² Ranges of geologic and displacement parameters for clastics, dolomite, and limestone lithologies for saline formations were used directly from Table 12 found in the IEA GHG (2009) report.

Table 6
 X_{10} and X_{90} values converted from P_{10} and P_{90} values from Eq. (7).

	Clastics		Dolomite		Limestone	
	X_{10}	X_{90}	X_{10}	X_{90}	X_{10}	X_{90}
$E_{An/At}$	-1.4	1.4	-1.4	1.4	-1.4	1.4
$E_{hn/hg}$	-1.32	1.15	-1.59	0.75	-1.90	0.49
$E_{\phi_e/\phi_{tot}}$	0.58	1.21	0.12	0.90	0.58	1.10
E_v	-1.66	-0.45	-1.05	-0.28	-0.71	0.28
E_d	-0.62	1.15	0.28	0.58	-0.99	-0.32

2006, 2008, 2010a). The equation, parameters, symbols, ranges, and description used to calculate efficiency for saline formations are summarized by Eq. (6) and Table 5.

$$E_{saline} = E_{An/At} E_{hn/hg} E_{\phi_e/\phi_{tot}} E_v E_d \tag{6}$$

Efficiency (E_{saline}) was estimated from the individual terms in Eq. (6) by Monte Carlo sampling. Each individual term in Eq. (6) is given by a fraction, p . Various parametric distribution functions, such as the normal, uniform, and lognormal, could be used to represent the distributions of the p 's. Currently, there is not enough data available to support assigning a specific distribution function to each of the individual terms in Eq. (6) at the regional and national scale designated for the US-DOE assessments. Since the p 's are fractions, they are constrained to the range between 0 and 1. Thus, the most appropriate distribution functions will be those that are constrained to the range between 0 and 1. Two distribution functions meeting this criterion and that were considered in this work are the beta distribution and the log-odds normal distribution. While both distributions are appropriate, the log-odds normal distribution, also known as the logistic-normal distribution (Aitchison and Shen, 1980), was chosen because of its ability to directly integrate the P_{10} and P_{90} ranges of geologic and displacement parameters provided by IEA GHG (2009) as presented in Table 5. It was assumed that the individual efficiency terms in Eq. (6) could all be represented using a log-odds normal distribution at the regional and national scale. From the limited data available (IEA GHG, 2009), all parameters were assumed to be independent as no significant correlation has been reported for these parameters at the regional or national level. However, parameters may be linked at the site-specific scale.

The log-odds normal distribution transforms a fraction, p , by Eq. (7) and assumes that the transformed variable is normally distributed.

$$X = \ln \left(\frac{p}{1-p} \right) \tag{7}$$

The distribution is given its name since the $p/(1-p)$ term in Eq. (7) is the “odds” for a fraction or probability p , therefore $\ln[p/(1-p)]$ is the “log odds”. The use of this distribution is referred to as the Log Odds Method when applied with the Monte Carlo sampling procedure (Devore, 2004). The transformed variable, X , is then normally distributed and sampled with appropriate Monte Carlo techniques for a normal random variable. Then, the X value is transformed back to the corresponding p value by Eq. (8), the inversion of Eq. (7):

$$p = \frac{1}{1 + e^{-X}} \tag{8}$$

Table 7
 μ_x and σ_x values calculated from X_{10} and X_{90} values from Eqs. (9) and (10).

	Clastics		Dolomite		Limestone	
	μ_x	σ_x	μ_x	σ_x	μ_x	σ_x
$E_{An/At}$	0	1.1	0	1.1	0	1.1
$E_{hn/hg}$	-0.09	0.97	-0.42	0.91	-0.71	0.93
$E_{\phi_e/\phi_{tot}}$	0.89	0.25	0.51	0.30	0.84	0.20
E_v	-1.05	0.47	-0.66	0.30	-0.21	0.39
E_d	0.27	0.69	0.43	0.11	-0.66	0.26

Since the relationship between p and X in Eqs. (7) and (8) is monotonic, X_{10} and X_{90} ranges of geologic and displacement parameters provided by IEA GHG (2009) can be computed directly from P_{10} and P_{90} ranges, respectively, using Eq. (7).

The Log Odds approach thus transforms ‘ p ’ values of a range into corresponding ‘ X ’ values of a range. This allows the mean and standard deviation of X to be determined from the X_{10} and X_{90} values. The mean and standard deviation of X fully specify its normal distribution, and these moments are then used as input parameters into the Monte Carlo sampling tools. The P_{10} and P_{90} values of the ranges presented in Table 5 were converted to X_{10} and X_{90} values by Eq. (7) and are shown in Table 6.

The mean (μ_x) and standard deviation (σ_x) are calculated from the X_{10} and X_{90} values using standard relationships between the percentiles and the moments of a normal distribution:

$$\sigma_x = \frac{X_{90} - X_{10}}{Z_{90} - Z_{10}} \tag{9}$$

$$\mu_x = X_{10} - \sigma_x Z_{10} \tag{10}$$

where Z_p is the P th percentile value of the standard normal distribution. In this case, Z_{10} equals -1.28 and Z_{90} equals 1.28 . Note that the standard deviation is computed first using Eq. (9), then this value is used to compute the mean in Eq. (10). The values of the moments for X computed using Eqs. (9) and (10) are shown in Table 7.

Monte Carlo sampling, using the commercial program GoldSim, was implemented using the mean (μ_x) and standard deviation (σ_x) values tabulated in Table 7 as input parameters. The respective X values are sampled using normal distributions with a sample size of 5000 iterations for each. The corresponding values of p are computed using Eq. (8), and the individual p values are multiplied together to determine the storage efficiency factor E as shown in Eq. (11):

$$E = p(E_{An/At})p(E_{hn/hg})p(E_{\phi_e/\phi_{tot}})p(E_v)p(E_d) \tag{11}$$

or equivalently,

$$E = \frac{1}{1 + e^{-X(E_{An/At})}} \frac{1}{1 + e^{-X(E_{hn/hg})}} \frac{1}{1 + e^{-X(E_{\phi_e/\phi_{tot}})}} \frac{1}{1 + e^{-X(E_v)}} \frac{1}{1 + e^{-X(E_d)}}$$

A value of E is thus obtained for each of the 5000 simulations, and the overall percentiles for the computed E are then estimated. Ranking from smallest to largest, the 500th result corresponds to P_{10} , the 2500th result corresponds to P_{50} , and the 4500th result corresponds to P_{90} . These results are shown in Table 8.

Table 8
Saline formation efficiency factors for geologic and displacement terms.

$E_{\text{saline}} = E_{\text{An/At}} E_{\text{hn/hg}} E_{\phi_e/\phi_{\text{tot}}} E_v E_d$			
Lithology	P_{10}	P_{50}	P_{90}
Clastics	0.51%	2.0%	5.4%
Dolomite	0.64%	2.2%	5.5%
Limestone	0.40%	1.5%	4.1%

The overall efficiency for saline formations ranges from 0.40 to 5.5% for the three different lithologies over the 10 and 90 percent probability range, respectively. These efficiency factors are based on documented ranges derived from oil and gas reservoirs and numerical simulations (IEA GHG, 2009). With previous versions of the Carbon Sequestration Atlas of the United States and Canada, geologic and displacement parameters were not based on documented ranges (DOE-NETL, 2006, 2008). These saline formation efficiency factors ranged between 1 and 4% over the P_{15} and P_{85} percent probability range (DOE-NETL, 2006, 2008). When undocumented ranges for saline formations for previous Carbon Sequestration Atlases of the United States and Canada (DOE-NETL, 2006, 2008) were applied using the Log Odds Method described here, the P_{10} , P_{50} , and P_{90} percent probability ranges were 0.51%, 2.0%, and 5.5%, respectively. While the two sets of input ranges generate similar overall efficiency factors for saline formations, the efficiency factors reported here are based on documented P_{10} and P_{90} ranges of geologic and displacement parameters for clastics, dolomite, and limestone lithologies and appropriate distribution functions, log-odds normal in this case, that are constrained to the range between 0 and 1 where previous efficiencies were not.

In the case where net-to-total area $E_{\text{An/At}}$, net-to-gross thickness $E_{\text{hn/hg}}$, and effective-to-total porosity $E_{\phi_e/\phi_{\text{tot}}}$ are known for a region or basin, the geologic efficiency values can be used directly in Eq. (6). In this instance, only the displacement efficiency factor is needed, which ranges between 7.4 and 26 percent over the 10 and 90 percent probability range (Table 9).

Overall, CO₂ storage resource estimates for saline formations are calculated from volumetric parameters (Eq. (2)) and efficiency factors (Eq. (6)) over the P_{10} , P_{50} , and P_{90} percent probability range (Tables 8 and 9).

$$G_{\text{CO}_2} = A_t h_g \phi_{\text{tot}} \rho E_{\text{saline}}$$

$$E_{\text{saline}} = E_{\text{An/At}} E_{\text{hn/hg}} E_{\phi_e/\phi_{\text{tot}}} E_v E_d$$

The probability estimates for G_{CO_2} in Eq. (2) are determined by applying the Monte Carlo procedure to estimate the quantiles (e.g., P_{10} , P_{50} and P_{90}) of E_{saline} in Eq. (6). The resulting P_{10} and P_{90} serve as nominal lower and upper bounds that demark a plausible range of efficiency factors, defined in a consistent probabilistic manner. If the 10th and 90th percentile values of the individual terms are properly specified for the targeted application, such as geologic storage, and the distributions for each term are independent and reasonably represented by the log-odds normal assumption, then the computed 10th and 90th percentile values for efficiency factors are properly estimated. However, because these limits are based on

Table 9
Saline formation efficiency factors for displacement terms.

$E_{\text{saline}} = E_v E_d^a$			
Lithology	P_{10}	P_{50}	P_{90}
Clastics	7.4%	14%	24%
Dolomite	16%	21%	26%
Limestone	10%	15%	21%

^a $E_{\text{An/At}}$, $E_{\text{hn/hg}}$, and $E_{\phi_e/\phi_{\text{tot}}}$ values are known directly.

a combination of data with varying quality and expert judgment, the P_{10} and P_{90} limits should be interpreted as general (rather than strictly mathematical) limits. That is, with reasonable 10th and 90th percentile limits chosen for each factor, the results provide reasonable 10th and 90th percentile limits for efficiency factors.

6.2. Efficiency of unmineable coal seams

As described in Section 5.3, CO₂ storage resource estimates for unmineable coal seams are calculated by Eq. (3).

$$G_{\text{CO}_2} = A h_g C_{s,\text{max}} \rho_{\text{CO}_2\text{std}} E_{\text{coal}}$$

For coal seams, the CO₂ storage efficiency factor is a function of geologic parameters such as area ($E_{\text{An/At}}$) and thickness ($E_{\text{hn/hg}}$) which reflect the percentage of volume that is amenable to CO₂ geologic storage and displacement efficiency components such as areal (E_A), vertical (E_L), gravity (E_g), and microscopic (E_d) which reflect the portion of a basin's or region's coal bulk volume with which CO₂ is expected to contact (Bachu et al., 2007; Doughty and Pruess, 2004; Koide et al., 1992; Shafeen et al., 2004; van der Meer, 1992). The effective-to-total porosity term is not applicable in coal seams. Eq. (12) describes CO₂ storage efficiency for coal seams:

$$E_{\text{coal}} = E_{\text{An/At}} E_{\text{hn/hg}} E_A E_L E_g E_d \tag{12}$$

The area ($E_{\text{An/At}}$) and thickness ($E_{\text{hn/hg}}$) terms gauge the portion of a basin's volume in which coal is present. The volumetric displacement terms (E_A , E_L , and E_g) identify the portion of the *in situ* coal volume for which the CO₂ is accessible. The microscopic displacement term (E_d) identifies the degree of CO₂ saturation (with respect to the maximum predicted by the Langmuir isotherm) within the CO₂-accessible deposit.

The net-to-total area $E_{\text{An/At}}$ ratio is the fraction of total basin or region area that has bulk coal present. This term accounts for known or suspected locations that are within a basin or region outline where a coal seam may be discontinuous. In the Illinois Basin, for example, there are sub-regions within the basin where sand channels have incised and replaced coal (DOE-NETL, 2008). The net to gross thickness $E_{\text{hn/hg}}$ ratio is the fraction of total coal seam thickness that has adsorptive capability. The areal displacement (E_A) efficiency is the fraction of the immediate area surrounding an injection well that can be contacted by CO₂. This term is influenced by areal geologic heterogeneity such as faults and permeability anisotropy. The vertical displacement (E_L) efficiency is the fraction of the vertical cross section or thickness with the volume defined by the area (A) that can be contacted by CO₂ from a single well. This term is influenced by variations in the cleat system within the coal. If one zone has higher permeability than other zones, the CO₂ will fill it quickly and leave the other zones with less or no CO₂. The gravity displacement (E_g) efficiency is the fraction of the net thickness that is contacted by CO₂ as a consequence of the density difference between CO₂ and the *in situ* water in the cleats. In other words, $1 - E_g$ is the portion of the net thickness not contacted by CO₂ because the CO₂ rises within the coal seam. The microscopic displacement (E_d) efficiency reflects the degree of saturation achievable for *in situ* coal compared with the theoretical maximum predicted by the CO₂ Langmuir Isotherm.

Because there is no documented database describing the statistical properties of coal seams, Monte Carlo simulations of storage efficiency for coal seams are based tentatively on coalbed methane (CBM) production and computer modeling observations (DOE-NETL, 2006, 2008, 2010a). In comparison with efficiency terms for saline formations, coal seam efficiency terms for area and thickness are increased because most coal basins are better defined than saline formations. Displacement efficiency terms for coal are also much higher than similar terms for porous media found in saline

Table 10
Parameters for unmineable coal seam efficiency.

Term	Symbol	P_{10}/P_{90} values	Description
Geologic terms used to define the entire basin or region pore volume			
Net-to-Total Area	$E_{An/At}$	0.6/0.8	Fraction of total basin or region area that has bulk coal present.
Net-to-Gross Thickness	$E_{hn/hg}$	0.75/0.90	Fraction of coal seam thickness that has adsorptive capability.
Displacement terms used to define the pore volume immediately surrounding a single well CO ₂ injector.			
Areal Displacement Efficiency	E_A	0.7/0.95	Fraction of the immediate area surrounding an injection well that can be contacted by CO ₂ .
Vertical Displacement Efficiency	E_L	0.8/0.95	Fraction of the vertical cross section (thickness), with the volume defined by the area (A) that can be contacted by a single well.
Gravity	E_g	0.9/1.0 ^a	Fraction of the net thickness that is contacted by CO ₂ as a consequence of the density difference between CO ₂ and the <i>in situ</i> water in the cleats.
Microscopic Displacement Efficiency	E_d	0.75/0.95	Reflects the degree of saturation achievable for <i>in situ</i> coal compared with the theoretical maximum predicted by the CO ₂ Langmuir Isotherm.

^a 0.9999999999999999 used due to inability to divide by zero when using Log Odds Method.

Table 11
Coal seam efficiency factors.

$E_{coal} = E_{An/At} E_{hn/hg} E_A E_L E_g E_d$		
P_{10}	P_{50}	P_{90}
21%	37%	48%

formations due to the adsorptive nature of coal. The gravity displacement term will likely be insignificant since coal seams are typically thinner than saline formations. Although it is known that coal swells in the presence of CO₂ and causes a reduction in permeability, coal swelling is not included in the efficiency equation at this time (Day et al., 2008b; Xie and Economides, 2009). The equation, parameters, symbols, ranges, and description used to calculate the storage efficiency factor for coal seams are summarized by Eq. (12) and Table 10.

Efficiency factors for coal seams were determined by using the Log Odds Method when applied with Monte Carlo sampling by Eqs. (7)–(11) as described in the Section 6.1. (Devore, 2004). The overall storage efficiency factor for coal seams ranges from 21 to 48 percent over the 10 and 90 percent probability range (Table 11). In the case where net-to-total area $E_{An/At}$ and net-to-gross thickness $E_{hn/hg}$ are known for an unmineable coal seam, the geologic efficiency values can be used directly in Eq. (12). In this instance, only the displacement efficiency factor is needed, which ranges between 39 and 77 percent over the 10 and 90 percent probability range (Table 12).

Overall, CO₂ storage resource estimates for unmineable coal seams are calculated from volumetric parameters (Eq. (3)) and efficiency factors (Eq. (12)), using the Monte Carlo procedure to determine the P_{10} , P_{50} , and P_{90} percent probability values for E_{coal} and the associated G_{CO_2} (results shown in Tables 11 and 12).

$$G_{CO_2} = A h_g C_{s,max} \rho_{s,max} E_{coal}$$

$$E_{coal} = E_{An/At} E_{hn/hg} E_A E_L E_g E_d$$

As before, the P_{10} and P_{90} values computed in this manner serve as nominal lower and upper bounds that demark a plausible range of efficiency factors, defined in a consistent probabilistic manner. If the 10th and 90th percentile values of the individual terms are properly specified for the targeted application, such as geologic storage, and the distributions for each term are independent and

Table 12
Coal seam efficiency factors for displacement terms.

$E_{coal} = E_A E_L E_g E_d^a$		
P_{10}	P_{50}	P_{90}
39%	64%	77%

^a $E_{An/At}$ and $E_{hn/hg}$ values known directly.

reasonably represented by the log-odds normal assumption, then the computed 10th and 90th percentile values for efficiency factors are properly estimated. However, because these limits are based on a combination of data with varying quality and expert judgment, the P_{10} and P_{90} limits should be interpreted as general (rather than strictly mathematical) limits. That is, with reasonable 10th and 90th percentile limits chosen for each factor, the results provide reasonable 10th and 90th percentile limits for efficiency factors.

7. Critical assessment of CO₂ storage resource calculations

7.1. Comparison of techniques for high-level storage efficiency factor calculations

In a recent report, IEA GHG (2009) developed another technique to estimate efficiency factors for CO₂ storage resource potential. They used numerical simulations to calculate efficiency factors for saline formations based on the ranges for geologic and displacement parameters they derived from field data for oil and gas reservoirs in the United States and relative permeability data published by Bennion and Bachu (2008). Efficiencies were calculated at the formation level and site-specific level. While the number of simulations needed to make these results statistically significant was not realized due to the computational time required by each simulation, their work provides estimates for low, mid, and high efficiency values for the different lithologies considered (IEA GHG, 2009).

We compared the efficiencies estimated for saline formations by IEA GHG (2009) with the efficiencies estimated by the US-DOE methodology. At the formation level, IEA GHG (2009) fixed the net-to-gross area $E_{An/At}$ and the net-to-gross thickness $E_{hn/hg}$ terms at the P_{50} values (see Table 5 for specific P_{50} values). Their storage efficiency coefficients ranged between 1.41 and 6.00% over the P_{10} and P_{90} percent probability range (Table 13). For comparison, efficiency factors using the Log Odds Method when applied with Monte Carlo sampling described here were calculated with the same fixed net-to-gross area $E_{An/At}$ and fixed net-to-gross thickness $E_{hn/hg}$ at the P_{50} values (Table 5). Efficiency factors ranged between 1.2 and 4.1% over the P_{10} and P_{90} percent probability range (Table 13).

At the site-specific scale, IEA GHG (2009) assumed that the net-to-gross area $E_{An/At}$ and the net-to-gross thickness $E_{hn/hg}$ terms were fixed at the P_{90} values (see Table 5 for specific P_{90} values). In this case, storage efficiency coefficients ranged between 4.24 and 14.92% over the P_{10} and P_{90} percent probability range (Table 14). For comparison, efficiency factors using the Log Odds Method when applied with Monte Carlo sampling described here were calculated with the same fixed net-to-gross area (A_n/A_t) and fixed net-to-gross thickness (h_n/h_g) at the P_{90} values (Table 5). Efficiency ranged between 3.1 and 10% over the P_{10} and P_{90} percent probability range (Table 14).

Table 13
Saline formation efficiency factors at the formation scale.

$E_{\text{saline}} = E_{\text{An/At}} E_{\text{hn/hg}} E_{\text{dpe/dtot}} E_v E_d$							
$E_{\text{An/At}}$ and $E_{\text{hn/hg}}$ terms fixed at P_{50} value							
Lithology	Numerical method ^a			Monte Carlo Method ^b			
	P_{10}	P_{50}	P_{90}	P_{10}	P_{50}	P_{90}	
Clastics	1.86%	2.70%	6.00%	1.2%	2.4%	4.1%	
Dolomite	2.58%	3.26%	5.54%	2.0%	2.7%	3.6%	
Limestone	1.41%	2.04%	3.27%	1.3%	2.0%	2.8%	

^a IEA GHG (2009).

^b This work.

The efficiency factors, estimated in this document using Monte Carlo sampling, were based on the use of a simplified analytical expression relating separate, independent factors to the total efficiency (e.g., Eq. (6)). Numerical simulations provide a more computationally rigorous approach to estimate efficiency factors as they require detailed geologic information that is typically not known at the regional and national level. The approach used for this assessment – analytical expression coupled with Monte Carlo sampling – requires minimal geologic input data, relying instead on statistical distributions that characterize geologic and displacement parameters of a formation at a large scale as derived from observations and experience in the oil and gas industries. In the context of estimating CO₂ storage resource estimates at the regional and national scale, Monte Carlo sampling in this study is appropriate for estimating efficiency for high-level initial resource estimates.

7.2. Open versus closed boundary condition assumptions for storage reservoir systems

Carbon dioxide storage resource estimates for this assessment, which reflect available pore volume of a formation that will be occupied by the injected CO₂, are based on volumetric methods where it is assumed that *in situ* fluids are either displaced from the formation or managed, for example, by production. Accordingly, storage resource estimates provide a high-level CO₂ storage estimate (as based on statistical properties that describe geologic and displacement parameters of a formation in Section 7.1). Capacity estimates, which reflect geologic storage potential when economic and regulatory issues are considered, will depend on detailed site-specific assessments of the reservoir, including factors that determine the degree to which the reservoir is opened or closed and how site-specific geology, economics, and regulations restrict management of *in situ* fluids. While no reservoir will behave like a completely open or closed system for individual injection locations, most formations will behave more like an open system than a closed one. Even in a fault-compartmentalized closed system that has shale confining units above and below, the small permeability of the shale will allow for pressure bleed-off which helps to reduce pres-

sure and increases capacity beyond the compressibility estimates (Birkholzer and Zhou, 2009; Birkholzer et al., 2009). Additionally, in those situations where a formation does behave like a closed system, it may be transformed into a more open system through the production of *in situ* fluids. Therefore, the US-DOE methodology assumes that the systems under study are open when estimating CO₂ storage resource potential (DOE-NETL, 2006, 2008, 2010a).

In open boundary systems, CO₂-induced displacement of storage reservoir fluids is expected to transfer the fluids to parts of the system outside of the area studied (i.e., outside the boundary). Certain considerations need to be made when calculating storage capacity estimates based on the open-system assumption. With open boundaries, displacement of *in situ* fluids may cause pressure changes in neighboring formations (Birkholzer and Zhou, 2009; Birkholzer et al., 2009; Leetaru et al., 2009; Nicot, 2008; Zhou et al., 2008). Potential impacts of fluid displacement depend upon the hydraulic connectivity between deep saline formations and other formations such as freshwater aquifers (Birkholzer and Zhou, 2009; Birkholzer et al., 2009; Leetaru et al., 2009; Zhou et al., 2008). Reported efficiency factors for saline formations with open boundaries range between 0.8 and 6% at the regional and national scale (Burruss et al., 2009; DOE-NETL, 2006, 2008, 2010a; Koide et al., 1992; Kopp et al., 2009a,b; Szulczewski and Juanes, 2009; van der Meer, 1995; van der Meer and Egberts, 2008a,b; van der Meer and Yavuz, 2009). These efficiencies are consistent with values reported here and within previous versions of the *Carbon Sequestration Atlas of the United States and Canada* (DOE-NETL, 2006, 2008).

In closed-boundary systems, the storage formation has defined non-permeable boundaries which may limit CO₂ storage due to potential pressure build-up in the formation (Birkholzer and Zhou, 2009; Birkholzer et al., 2009; Economides and Ehlig-Economides, 2009; Leetaru et al., 2009; Xie and Economides, 2009; Zhou et al., 2008). As in open systems, excess pressure in a closed system must be managed to avoid damage that could result in a breach of seal integrity (Economides and Ehlig-Economides, 2009; van der Meer, 1992, 1993, 1995; van der Meer and Egberts, 2008a,b; van der Meer and Yavuz, 2009; Xie and Economides, 2009). The potential for CO₂ storage in a closed system comes mainly from the pore volume increase due to compression of reservoir fluids and rocks

Table 14
Saline formation efficiency factors at the site-specific scale.

$E_{\text{saline}} = E_{\text{An/At}} E_{\text{hn/hg}} E_{\text{dpe/dtot}} E_v E_d$							
$E_{\text{An/At}}$ and $E_{\text{hn/hg}}$ terms fixed at P_{90} value							
Lithology	Numerical method ^a			Monte Carlo method ^b			
	P_{10}	P_{50}	P_{90}	P_{10}	P_{50}	P_{90}	
Clastics	4.62%	6.79%	14.92%	3.1%	6.1%	10%	
Dolomite	6.57%	7.91%	14.92%	5.1%	6.9%	9.2%	
Limestone	4.24%	6.13%	9.82%	3.5%	5.2%	7.3%	

^a IEA GHG (2009).

^b This work.

at the higher pressure. Reported efficiency factors for saline formations with closed boundaries range between 0.35 and 1% near the CO₂ injection well (Economides and Ehlig-Economides, 2009; Gorecki et al., 2009b; Okwen et al., 2010; van der Meer, 1992, 1993, 1995; van der Meer and Egberts, 2008a,b; van der Meer and Yavuz, 2009; Xie and Economides, 2009; Zhou et al., 2008). Hence, the assumption of closed reservoirs would lower total efficiencies by a factor of 1/3 to 1/6. However, if one only includes compressibility of fluid and formation, and not bleed-off pressure, then efficiency factors for saline formations with closed boundaries will be conservative (Birkholzer and Zhou, 2009; Birkholzer et al., 2009).

7.3. Role of CO₂ physicochemical properties on storage resource and capacity estimates

In the US-DOE methodology, CO₂ dissolution in brine and mineral precipitation effects are not taken into account when calculating saline formation CO₂ storage resource estimates. The dissolution of injected CO₂ into brine and carbonate mineral formation reactions are complex processes that are dependent on the temperature, pressure, and brine composition within a formation, as well as the effectiveness of the contact between free phase CO₂, the formation brine and, subsequently, the minerals in the formation strata (Bachu et al., 2007). The amount of time required for effective CO₂ dissolution and carbonate mineral formation is not well understood. Current estimates indicate that mineral precipitation in brines under typical reservoir conditions is likely to be on the order of hundreds to thousands of years, however, it is expected that CO₂ dissolution occurs on a shorter time scale (Ennis-King and Paterson, 2003; Gupta et al., 2004; van der Meer and van Wees, 2006). Ongoing research will help enhance our understanding of the best practice to account for CO₂ dissolution and carbonate mineral formation in CO₂ storage resource estimates.

8. Summary and conclusions

The US-DOE methodology for estimating CO₂ storage resource potential for geologic carbon dioxide (CO₂) storage is presented in detail. Methodology is provided for determining CO₂ storage resource estimates for three types of geologic formations: oil/gas reservoirs, saline formations, and unmineable coal seams. These CO₂ storage resource estimates are based on physically accessible CO₂ storage pore volume in formations, and on the assumption that the storage reservoirs are open systems in which the *in situ* fluids will either be displaced from the injection zone or managed. Economic and regulatory constraints are not considered. This methodology is intended to produce high-level CO₂ resource estimates of potential geologic storage in the United States and Canada at the regional and national scale. At this scale, the estimates of CO₂ geologic storage have a high degree of uncertainty. Because of this uncertainty, estimates are not intended to be used as a substitute for site-specific characterization and assessment. As CO₂ storage sites move through the site characterization process, additional site-specific data will be collected and analyzed, reducing uncertainty. Incorporation of these site-specific data will allow for refinement of CO₂ storage resource estimates and development of CO₂ storage capacities by future potential commercial project developers. These resource estimates are intended for use by external users such as Regional Carbon Sequestration Partnerships (RCSPs), future project developers, and governmental entities for high-level assessments of potential CO₂ storage reservoirs in the United States and Canada at the regional and national scale, however, the methodology is general enough that it could be applied for initial screening assessments in other locations.

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