International Journal of Greenhouse Gas Control 91 (2019) 102808

Contents lists available at ScienceDirect

International Journal of Greenhouse Gas Control

journal homepage: www.elsevier.com/locate/ijggc

A guideline for appropriate application of vertically-integrated modeling approaches for geologic carbon storage modeling

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ARTICLE INFO

Keywords:
Geologic carbon storage modeling
Model complexity
Decision criteria
Model choice

ABSTRACT

Mathematical modeling is an essential tool for answering questions related to geologic carbon storage (GCS). The choice of modeling approach depends on the type of questions being asked. In this paper we discuss a series of approaches with a hierarchical complexity including vertically-integrated single-phase flow approaches, vertically-integrated multi-phase flow approaches (with and without vertical equilibrium assumption), three-dimensional multi-phase flow approaches, and fully-coupled multi-phase flow approaches that couple flow with geochemistry and/or geomechanics. Three spatial scales are used to categorize the questions to be addressed by modeling: regional scale (encompasses CO_2 plume extent and majority of area of pressure impact of one or more injection operations), site scale (includes the CO_2 plume extent and some of the area impacted by the pressure increase of a single injection site), and well scale (the immediate vicinity of an injection well). A set of guidelines is developed to help modelers choose the most appropriate modeling approach, and show when simpler modeling approaches may be the better choice. Vertically-integrated single-phase flow models are the most appropriate choice at both the site and regional scales, if the pressure impact outside of the CO_2 plume is of interest. Vertically-integrated multi-phase flow models should be chosen at the regional scale, if the locations of CO_2 plumes are of interest, and at the site scale if vertical segregation of CO_2 and brine is fast or vertical heterogeneity in properties can be presented by distinct, continuous layers. Three-dimensional multi-phase flow models are the appropriate choice at the well and site scales for cases with significant vertical flow components of CO_2 and brine. Fully-coupled multi-phase flow models should only be chosen if pore-space alteration through geochemistry or geomechanics feeds back to fluid flow.

1. Introduction

Carbon capture and storage (CCS) is a technology for mitigating anthropogenic carbon dioxide (CO_2) emissions from large stationary sources, such as fossil-fuel burning power plants. CO_2 is captured at the source and injected into the subsurface for permanent storage, instead of being vented to the atmosphere (Metz et al., 2005). In order to significantly reduce emissions a volume of CO_2 on the same order of magnitude as current world-wide oil production would need to be stored (Celia et al., 2015). Deep saline aquifers have been determined to be the most likely storage formations (Metz et al., 2005) due to their high storage capacity and injectivity (i.e., their capacity to sustain large CO_2 injection rates without fracturing the overlying formations). Depleted oil fields are also being targeted as additional oil may be produced by injecting CO_2 through a process called CO_2 enhanced oil recovery (CO_2-EOR). While carbon capture and transport to a suitable storage sites come with their own challenges, this discussion focuses on geologic carbon storage (GCS), the storage component of CCS.

During a GCS operation CO_2 is injected into a storage formation for permanent storage. Due to the large density difference between the injected CO_2 and the resident brine (CO_2 is about 250–1000 kg/m^3 less dense than brine; in other words brine is a factor of 1.25–5 times more dense than CO_2) (Metz et al., 2005), CO_2 migrates vertically due to buoyancy, so that a low-permeability caprock formation needs to overlie the injection formation, providing for structural trapping of the injected CO_2. In addition to structural trapping, additional important mechanisms are: residual trapping (i.e., CO_2 being held in place through capillary forces), dissolution trapping (i.e., CO_2 dissolving into brine), and mineral trapping (i.e., CO_2 precipitating in the pore space as carbonate rock). Migration of brine may be important as it has the potential to negatively impact underground sources of drinking water (USDW). Furthermore, injection of CO_2 increases the pressure in the

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https://doi.org/10.1016/j.ijggc.2019.102808
Received 25 January 2019; Received in revised form 14 July 2019; Accepted 6 August 2019

subsurface, potentially leading to seismic events that have impacts at the surface or on other subsurface activities and potentially create leakage pathways for CO_2.

CO_2 needs to be stored effectively (i.e., no or very little CO_2 leakage to the shallow subsurface or atmosphere) and safely (i.e., no deleterious impacts on subsurface or surface activities) for a GCS operation to be successful. Several questions need to be answered to address the safety and effectiveness of GCS:

- Where do the injected CO_2 and resident brine migrate to?
- What is the injection induced pressure response in the injection formation and adjacent formations?
- How much and at what injection rate can CO_2 be stored (i.e., dynamic storage capacity)?
- In what form (free-phase, capillary trapped phase, dissolved in brine, precipitated) is CO_2 being stored and how does this proportioning evolve over time?
- How does the GCS operation impact other activities at the surface and in the subsurface?

Mathematical modeling is usually used to answer these questions. As a model is an approximation of reality, the modeler needs to choose which processes to include and which to neglect. In GCS CO_2 is usually injected in its supercritical form leading to a two-phase (CO_2-rich phase and brine-rich aqueous phase) flow system in which viscous, buoyancy and capillary forces determine the migration of the two fluids. Brine may evaporate into the CO_2 phase and CO_2 may dissolve into the brine phase. The fluid properties (i.e., density and viscosity) can change with pressure, temperature and fluid composition. Constituents in the two phases and the rock matrix may undergo chemical reactions, potentially leading to dissolution of the rock matrix or precipitation of new minerals and an accompanying alteration of the pore space. The injection-induced pressure response changes the stress state in the subsurface, leading to an alteration of the pore space through seismic events (e.g., creation or reactivation of fractures and faults) or expansion (e.g., surface uplift). All these processes may play significant roles during GCS operations, and modelers usually need to choose which of them to include in a model. Most of the discussion in this paper is focused on modeling fluid migration, so that geochemistry and geomechanics are only included if they lead to significant changes in rock parameters (e.g., porosity and permeability). However, geochemistry and geomechanics are needed when tracer breakthrough or surface uplift are used for monitoring, or when investigating induced seismicity.

While flow processes at the pore scale need to be understood, for any practical calculations, GCS modeling is conducted at the continuum scale. For instance, snap-off at the pore scale is treated as residual saturation at the continuum scale, and changes in the pore size due to dissolution/precipitation are reflected in changes of porosity and permeability. Relying on continuum scale models sets the lower bound for the length scale of GCS models to be on the order of centimeters. On the other hand, some questions may lead to models with spatial scales of hundreds of kilometers (e.g., interference of GCS operations in a basin-wide deployment of GCS). In this paper, we define three spatial scales, termed regional, site and well scale. The regional scale encompasses the CO_2 plumes and the majority of the pressure response for one or more GCS operations (typically on the order of tens to hundreds of kilometers). The next smaller scale is the site scale which includes the CO_2 plume and some of the pressure response of a single GCS operation (typically on the order of hundreds of meters to tens of kilometers). The well scale, the smallest of the three, captures processes in the direct vicinity of the injection well (typically tens of centimeters to several tens of meters). Modeling of flow in a single fracture is also considered to be at the well scale, although the aperture scale is typically on the order of millimeters or smaller.

There are also two ranges of time scales that are significant for GCS modeling. The first one relates to the form of CO_2: free-phase (gas phase), dissolved (liquid phase) or mineral (solid phase). CO_2 is injected as free-phase, some of which can dissolve into brine and potentially precipitate. When free-phase CO_2 comes in contact with brine, the dissolution processes is very fast (often considered instantaneous) in the direct vicinity of the CO_2-brine interface. Direct contact only occurs within the CO_2 plume, limiting the amount of CO_2 that can dissolve into brine over this short time scale. Density driven mixing – which occurs because brine with dissolved CO_2 is denser than pure brine – increases the amount of CO_2 that can dissolve and leads to transient mixing (e.g., Emami-Meybodi et al., 2015; Green and Ennis-King, 2018) over longer time scales, often tens to hundreds of years. The precipitation time scale is much longer, on the order of hundreds to thousands of years (e.g., Hitchon et al., 1999). However, the precipitation rates seem to depend strongly on the host rock, as experiments in basalts have shown precipitation time scales on the order of months (Matter et al., 2016), rather than the hundreds of years estimated for siliciclastic rocks. A second time scale is related to the time it takes for CO_2 and brine to segregate in the vertical direction due to buoyancy. The segregation time scale can be estimated based on the density difference between CO_2 and brine, the permeability and thickness of the formation, and other parameters (Nordbotten and Dahle, 2011). Because of the relative permeability effect, while much of the CO_2 may segregate relatively quickly, the time can increase significantly as the brine saturation approaches its residual value (Becker et al., 2017). As such, a practical definition of segregation time needs to be adopted (Becker et al., 2017).

Considering the relevant processes and length and time scales involved, a modeler needs to choose an appropriate modeling approach, while also taking into account the availability of data and computational resources. Modeling approaches applicable to GCS range in complexity – and data intensity and computational demands – from semi-analytical single-phase models to fully-coupled three-dimensional approaches that include non-isothermal effects, geomechanics and geochemistry along with fluid flow. Following is a brief description of the relevant modeling approaches going from least complex to most complex; for more detailed descriptions refer to Bandilla et al. (2015) (Fig. 1).

In single-phase models CO_2 injection is modeled as a volume-equivalent injection of brine (e.g., Huang et al., 2014; Nicot, 2008), eliminating the complexities introduced by multi-phase flow. Single-phase models are based on a combination of mass balance and Darcy's law equations (e.g., Nordbotten and Celia, 2012). The governing equations are solved numerically to determine the pressure distribution (the primary unknown) in the model domain. For cases with negligible vertical flow in an aquifer (e.g., large lateral extent compared to aquifer

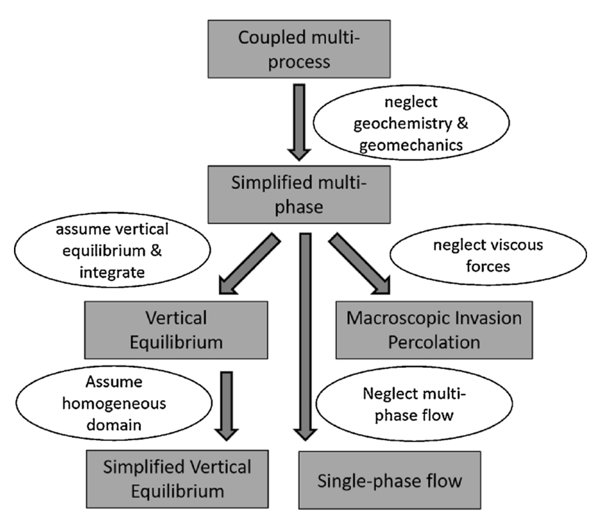

Fig. 1. Hierarchy of modeling approaches. Reproduced from Bandilla et al. (2015) with permission from Wiley.

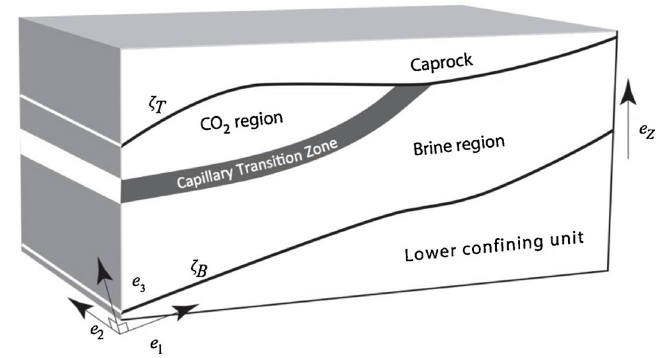

Fig. 2. Conceptual sketch of CO_2 storage formation. Reproduced from Nordbotten and Celia (2012) with permission from Wiley.

thickness), vertically-integrated governing equations can be used, leading to a set of two-dimensional equations that is solved numerically or semi-analytically for cases with simple geometries and homogeneous aquifer properties (e.g., Zhou et al., 2009).

Vertically-integrated vertical-equilibrium multi-phase flow (VE) models represent the next level of complexity for GCS models. VE models are based on a set of two dimensional equations, derived by integrating the three-dimensional governing equations of multi-phase flow in the direction perpendicular to the bedding plane of the aquifer (Fig. 2). The vertical phase distributions – needed to compute the vertically-integrated relative permeabilities – are calculated based on the vertical equilibrium assumption, which assumes that CO_2 and brine maintain pressure equilibrium (hydrostatic) in the vertical direction (Fig. 3). The resulting set of vertically-integrated equations is then solved numerically for the four primary unknowns: the two reference phase pressures and the two depth-averaged phase saturations. For domains with simple geometries and constant aquifer and fluid properties along with negligible capillary pressure, the set of vertically-integrated governing equations can be solved semi-analytically. For more details on VE models for GCS the reader is referred to Nordbotten and Celia (2012).

While many vertically-integrated modeling approaches rely on the vertical equilibrium assumption to reconstruct the phase saturation profiles, the vertically-integrated dynamic-reconstruction multi-phase flow approach (DR) relaxes the VE assumption (Guo et al., 2014, 2016a). In the DR approach, the vertical segregation of CO_2 and brine is modeled by solving a dynamic vertical fractional flow equation, after solving the two-dimensional vertically-integrated equations for depth-averaged phase saturations and reference phase pressures at every numerical time step. Like the VE approach, the DR approach can be seen as a multi-scale approach, with the lateral migration corresponding to the coarse scale and the vertical dynamics being the fine scale.

The next more complex modeling approach is the fully-resolved three-dimensional multi-phase flow (3D multi-phase flow) approach. In the 3D multi-phase flow approach the three-dimensional governing equations for multi-phase flow are solved numerically, resulting in a three-dimensional spatial distribution of the primary unknowns: the two phase saturations and the phase pressures. In other words, no reconstruction of pressures and saturations is necessary, because the 3D multi-phase flow modeling approach directly resolves the vertical direction. This modeling approach is the most commonly used approach for GCS modeling and forms the foundation for widely used simulators such as TOUGH2 (Pruess et al., 1999; Zhang et al., 2008), STOMP (White and Oostrom, 2006; White et al., 2012), PFLOTRAN (www.pflotran.org), FEHM (fehm.lanl.gov), DuMu^x (Flemisch et al., 2011), ECLIPSE (Schlumberger, 2010), and CMG-GEM (Group, 2010).

The most complex modeling approach is the fully coupled approach, where governing equations of three-dimensional multi-phase flow are solved together with equations representing processes such as geomechanics, geochemistry, and/or energy transport. Directly coupling solutions for the different processes can be quite complex, so that it is common to link separate models for the processes to a multi-phase flow simulator. For instance, when solving for rock deformation due to CO_2 injection, a multi-phase flow simulator can be linked to an independent geomechanics simulator with updated pressures and deformations passed between the two simulators at each time step (e.g., Rinaldi and Rutqvist, 2013). It should be noted that the multi-phase flow simulator used in fully-coupled approaches does not need to be a three-dimensional model, as Bjørnarå et al. (2016) developed a coupled flow and geomechanics model where both flow and deformation in the injection formation are based on vertically-integrated equations.

A recent development is the adaptation of dual-domain models to the GCS context for CO_2 storage in fractured aquifers. In this approach, the rock matrix and the fractures are treated as separate flow domains which are coupled through the exchange of mass between the two domains. The fractures are generally modeled as a continuous porous medium; several representations for the rock matrix have been used. The most common representations are sugar cube, matchstick, multiple interacting continua (MINC), and dual-permeability. While the dual-domain concept has a rich application history in petroleum, contaminant transport and geothermal research, mass transfer functions for the GCS context have only been developed recently. March et al. (2016) and March et al. (2018) developed mass transfer functions to specifically represent the exchange of CO_2 and brine between fractures and the rock matrix for 3D multi-phase flow models. Tao et al. (2019) developed a vertically-integrated dual-porosity approach by coupling a vertically-integrated model for the fractures to a sugar-cube model for the rock matrix.

There are current developments hybridizing different modeling approaches for the context of GCS. For example, Becker et al. (2018)

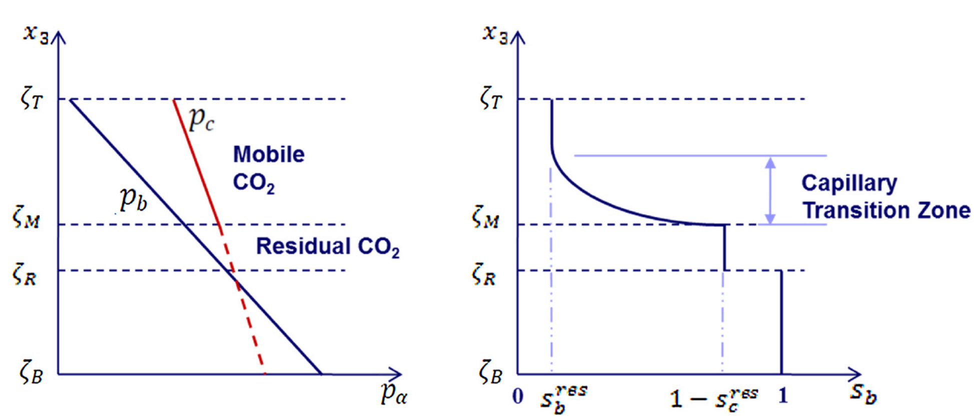

Fig. 3. Brine (p_b) and CO_2 (p_c) pressure profiles at vertical equilibrium (left), and associated brine saturation (right). Reproduced from Celia et al. (2015) with permission from Wiley.

and Møyner et al. (2018) combine a 3D multi-phase flow model with a VE model, so that the VE model covers parts of the domain where the vertical equilibrium assumption is valid, while the 3D multi-phase flow model covers parts with significant vertical flow. Hybrid approaches have the potential to be especially useful for cases bridging multiple scales. For instance, vertical flow dynamics close to the injection well could be modeled by a 3D model, while the rest of the CO_2 plume and beyond could be modeled by a VE model. The conditions under which the separate parts (e.g., single-phase, 3D, VE, …) are appropriate is discussed later in this article, but additional research is necessary to determine conditions where hybrid models are more appropriate, than utilizing a single approach.

The modeling approaches mentioned above all have in common that they are based on a combination of fluid mass balance equations and Darcy's law, however other modeling concepts have been applied to GCS modeling as well. For instance, a macroscopic invasion percolation modeling approach was used to simulate CO_2 migration at the Sleipner and In Salah sites (Cavanagh and Ringrose, 2011; Cavanagh and Haszeldine, 2014). However, the macroscopic invasion percolation modeling approach was not shown to be an accurate modeling approach in those studies, and is therefore not discussed here. Surrogate modeling approaches such as reduced order models (ROMs) are increasingly being applied to GCS modeling due to their low computational cost once constructed and ease of coupling diverse processes (e.g., Bromhal et al., 2014; Jin and Durlofsky, 2018; Pawar et al., 2016; Shahkarami et al., 2014; Zhang et al., 2016b). However, most ROMs require modeling GCS using one of the modeling approaches mentioned above to construct the surrogate model. Thus, a discussion of the applicability of surrogate modeling approaches is beyond the scope of this study, although, once constructed, ROMs can be very powerful tools. It should be noted, that "reduced order" refers to the use of surrogate models (i.e., reduction in conceptualization) and not the reduction of dimensionality through integration along one of the spatial directions as in the VE models (i.e., going from a three-dimensional model to a two-dimensional model).

In this paper we first describe the modeling approaches mentioned above and discuss their application to GCS modeling at different spatial scales based on example applications. While the time scales also have important implications on modeling approach choice, this paper is structured based on spatial scales, and time scales are taken into account implicitly. For instance, the impact of the vertical segregation time scale is taken into account through the proxy of intrinsic permeability and the long time scales related to precipitation in some formations is taken into account by neglecting precipitation for question answered on shorter time scales. The description of modeling approaches is followed by a set of guidelines to help modelers choose the most appropriate modeling approach based on the question(s) asked and the conditions at the site. The goal of this article is to highlight conditions and questions where vertically integrated models may be the most appropriate tool and to motivate model users and developers to look beyond the modeling approaches they most commonly use.

2. Application of modeling approaches

In this section we describe the different modeling approaches, solution methods, the scales they have been applied to, and lessons that have been learned from the application of the approaches to GCS sites. The approaches are ordered from least complex to most complex.

2.1. Single-phase models

In single-phase models volume-equivalent brine injection (i.e., a volume of brine equivalent to the volume of CO_2 injection to be modeled) is used to approximate GCS operations. The approach is based on a mass balance equation for brine along with brine fluxes represented by Darcy's law. The impact of brine compressibility and deformation of the rock matrix through pressure changes is usually represented by a storativity term. Depending on the formulation, the primary variable is either pressure or hydraulic head. The resulting set of three-dimensional governing equations is solved numerically (e.g., Harbaugh, 2005). For conditions where vertical flow is negligible (e.g., when the lateral extent is much larger than the vertical extent) the governing equations can be integrated in the vertical direction assuming zero resistance to flow in the vertical direction. The resulting set of vertically integrated equations is solved numerically. For aquifers with simple geometries and constant aquifer properties, the vertically integrated equations can also be solved analytically, leading to well-known solutions, such as the Theis solution (Theis, 1935).

In the context of GCS modeling, single-phase models are typically used at the regional scale to investigate the pressure response. At this large scale the impact of multi-phase flow effects becomes negligible, because CO_2 only occupies a very small portion of the model domain. Huang et al. (2014) investigated the impact of hypothetical GCS operations in the Basal Cambrian Aquifer in Canada by modeling the entire basin ($\sim 800{,}000\ km^2$) using both single-phase and multi-phase vertically-integrated models. They found that results from the single-phase and multi-phase models compared well to each other when taking into account the spatial variability of formation properties (e.g., permeability, thickness), but that a superposition of semi-analytical solutions – both single-phase and multi-phase – were not able to give accurate results, due to their assumption of constant formation properties (Fig. 4). Also, Nicot (2008) investigated the impact of GCS operations in the Gulf Coast Basin (Texas, USA) on up-dip fresh water resources based on a three dimensional single-phase model covering about $80{,}000\ km^2$. While the model predicted an increased groundwater table in the outcrop areas of about 1 m, the water quality of the freshwater areas was not impacted. Cihan et al. (2013) investigated injection-induced brine leakage through both the caprock and concentrated leakage pathways (e.g., abandoned wells and conductive faults) using a semi-analytical solution for vertically-integrated single-phase flow in stacked formations. A comparison to a three-dimensional multi-phase flow simulator showed good agreement, especially during the injection phase. Poorer agreement during the post-injection phase was attributed to the difference in effective compressibility of brine as compared to a combination of brine and CO_2 for the multi-phase case (Cihan et al., 2013). Kissinger et al., (2017) modeled vertical brine migration through faults using both sing-phase and multi-phase three-dimensional models. They found that while accurately presenting changing salinities was important, multi-phase flow effects had little impact on brine leakage rates as the faults were outside of the CO_2 plume. Lastly, Zhang et al. (2013) used a numerical single-phase flow model to investigate the impact of basal faults in transferring pressure into the crystalline basement, increasing the potential for induced seismicity. They benchmarked their single-phase flow model against published multi-phase flow results (Birkholzer et al., 2009) and found a good match between the two modeling approaches.

2.2. Vertically-integrated vertical equilibrium multi-phase flow models

Vertically-integrated vertical equilibrium multi-phase flow (VE) models follow the next more complex modeling approach. They are more complex than single-phase models, as they include multi-phase flow effects. VE models are based on the vertically-integrated mass balance equations for CO_2 and brine, along with a vertically-integrated version of Darcy's law to describe the vertically-integrated phase fluxes, relationships between phase saturation, capillary pressure and relative permeability, and constitutive relationships for the fluid phases. The geometric constraint that the entire pore space is filled by the two fluids is used to close the system of equations (e.g., Nordbotten and Celia, 2012). The resulting system of two-dimensional equations can then be solved either semi-analytically or numerically, with the two depth-averaged phase saturations and the two reference phase pressures as the

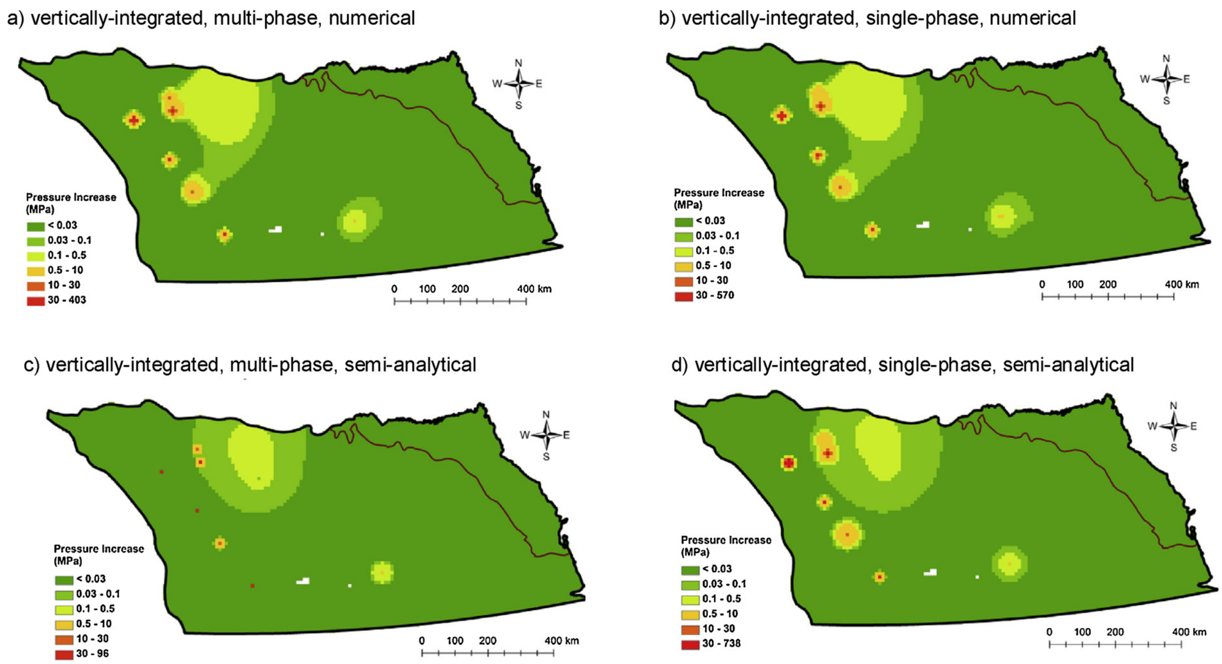

Fig. 4. Comparison of simulated injection-induced pressure increase in the Basal Cambrian Aquifer based on four vertically-integrated modeling approaches: (a) multi-phase, numerical, (b) single-phase, numerical, (c) multi-phase, semi-analytical, and (d) single-phase semi-analytical. Modified from Huang et al. (2014) with permission from Elsevier.

primary unknowns. However, in order to evaluate the integrated relative permeabilities, the vertical phase saturation profiles need to be reconstructed based on the depth-averaged phase saturations. In VE models it is assumed that CO_2 and brine segregate instantaneously in the vertical direction due to buoyancy. This leads to pressure equilibrium in the vertical direction (i.e., both phases have "hydrostatic" pressure profiles (Fig. 3)), and this assumption is termed the vertical equilibrium assumption.

Residual trapping can be represented in VE models by considering all CO_2 below the residual depth averaged CO_2 saturation as immobile once brine imbibes into the CO_2 plume (Gasda et al., 2009). Gasda et al. (2011) developed a VE sharp-interface model that included dissolution trapping by allowing for CO_2 dissolution into residual brine within the CO_2 plume as well as dissolution from the CO_2 plume into brine below the sharp interface. While dissolution into residual brine is based on equilibrium partitioning, the dissolution across the macroscopic sharp interface is governed by gravity-enhanced convective mixing.

Multiple VE models, separated by caprocks, may be stacked on top of each other leading to quasi-three-dimensional models, for instance to simulate a sedimentary stack of formations. In these quasi-three-dimensional VE models, adjacent VE layers are connected to each other through diffuse leakage of brine through the caprock and leakage along concentrated leakage pathways (Bandilla et al., 2012). For cases with constant formation and fluid properties, a negligible capillary transition zone (i.e., a macroscopic sharp interface between CO_2 and brine), and a laterally infinite domain, the vertically-integrated multi-phase flow equations can be solved semi-analytically, with the thickness of the CO_2 plume and pressure at the bottom of the formation being the primary unknowns (e.g., Guo et al., 2016c; Lyle et al., 2005; MacMinn et al., 2010; Nordbotten and Celia, 2006; Pegler et al., 2014; Zheng et al., 2015). Guo et al. (2016b) examined different semi-analytical solutions for GCS modeling to determine regions in the parameter space where those solutions are applicable to GCS related question (Fig. 5).

The main limitation of VE models is that the vertical equilibrium assumption needs to be valid. Court et al. (2012) found that the vertical equilibrium assumption is likely to be valid for formations with permeabilities larger than ~100 mD (mD = 10^{-3} Darcy ≈ $10^{-15}\,m^2$) for injection rates and formation thicknesses typical for GCS sites.

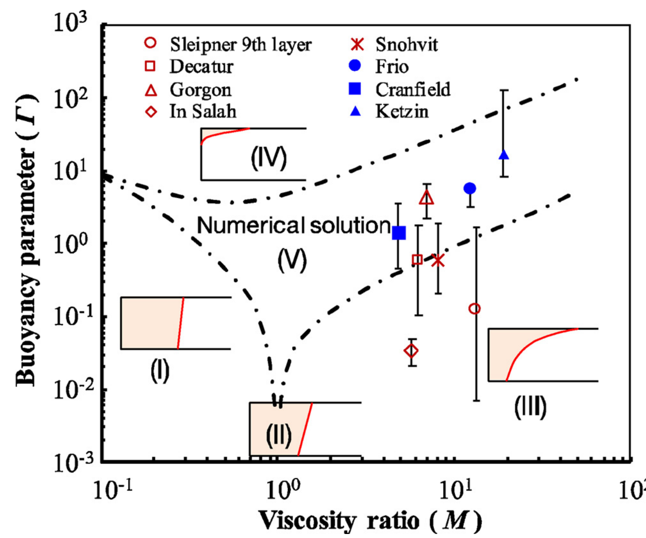

Fig. 5. Applicability of different semi-analytical solutions based on flow regimes. The viscosity ratio is defined as $M = \mu_b/\mu_c$, and the buoyancy parameter $\Gamma = 2\pi\Delta\rho gkh_0^2/(\mu_b q)$ represents the relative importance of buoyancy and the force from fluid injection. μ_b and μ_c are the viscosities of brine and CO_2, respectively; $\Delta\rho$ is the density difference between CO_2 and brine; k is the permeability of aquifer; h_0 is the thickness of the aquifer; q is the volumetric injection rate; g is the magnitude of gravity acceleration. Modified from Guo et al. (2016b) with permission from Elsevier.

However, Becker et al. (2017) found that even in highly permeable formations final drainage of brine out of the CO_2 plume may be very slow due to very low relative brine permeability at high CO_2 saturations. They then modified the VE model by introducing the concept of pseudo-residual brine saturation, where the residual brine saturation value used in the VE model decreases dynamically with time to capture the slow final drainage process, thus allowing brine saturation values above residual in the VE model.

VE models have been applied to GCS modelling at both the site and

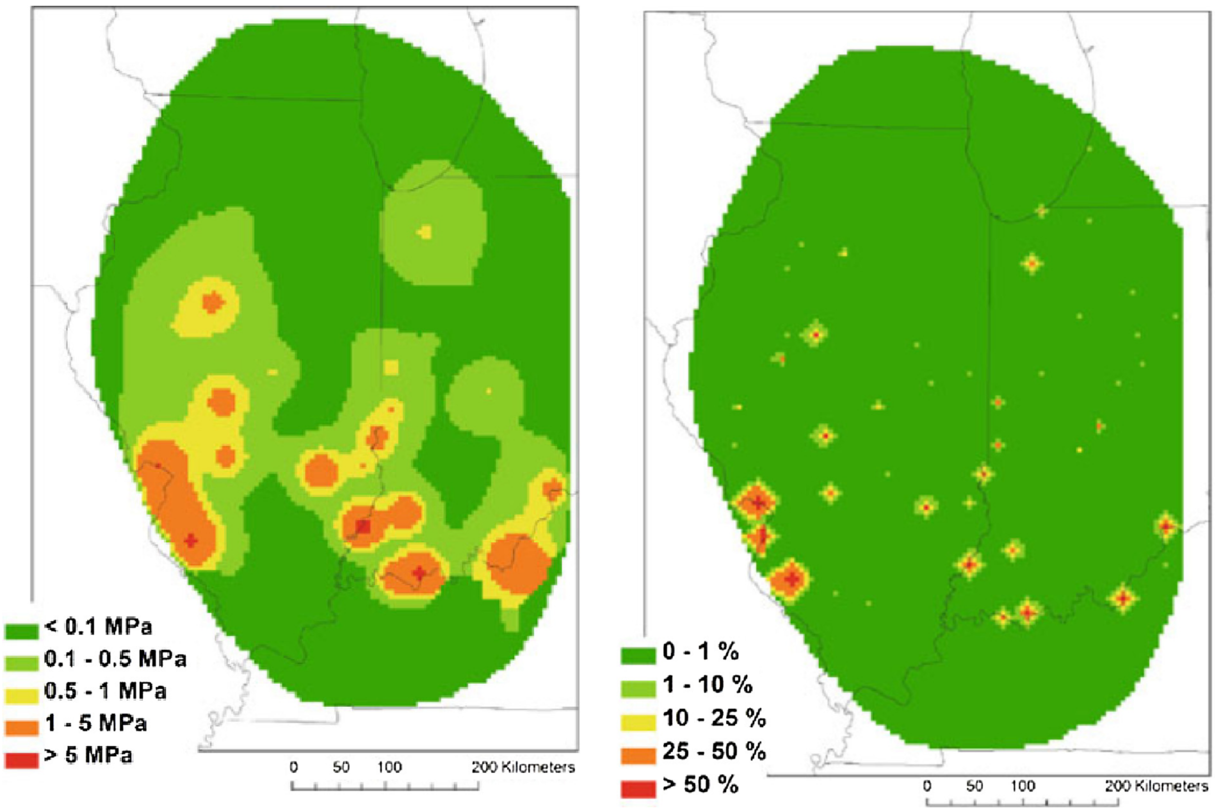

Fig. 6. Predicted results for a hypothetical industrial-scale CO_2 injection scenario in the Mount Simon Sandstone based on a VE model: pressure increase (left) and CO_2 saturation (right). Reprinted by permission from Springer Nature: Bandilla et al. (2012).

regional scales. For instance, Person et al. (2010) and Bandilla et al. (2012) used numerical VE models at the regional scale (230,000 km^2 and 300,000 km^2, respectively) to investigate hypothetical scenarios of industrial-scale deployment of GCS in the Illinois Basin (USA) (Fig. 6) and their results compared well to results from a study using a three-dimensional multi-phase flow model (Zhou et al., 2010). Gasda et al. (2012) used a regional-scale numerical VE model of the Johansen formation (Norway, 2100 km^2) to investigate long-term storage safety by tracking mobile, residually trapped and dissolved CO_2 over 1000 years (50 years of injection). Examples for VE models being applied at the site scale include two studies investigating CO_2 migration in the 9th layer at the Sleipner site (Norway). Both Nilsen et al. (2011) and Bandilla et al. (2014) compared numerical VE models to numerical three-dimensional multi-phase flow simulators and found good agreement between the two approaches, although neither approach was able to capture some of the lateral migration pathways seen from seismic imaging in the field. Hypothetical site-scale VE models based on permeability heterogeneity patterns – both laterally and vertically – observed at the Ketzin injection site (Germany) have also been used to determine the applicability of numerical VE models for such cases by comparison to three-dimensional multi-phase flow simulators (Bandilla et al., 2017). In an additional example, Cihan et al. (2015) coupled a numerical VE model with a heuristic optimization approach to find optimal pumping rates for keeping the pressure response at a fault below a threshold.

Semi-analytical VE models have been applied to GCS modeling. Szulczewski et al. (2012) used a semi-analytical VE model that included residual trapping and CO_2 dissolution to estimate the storage capacity of sloping saline formations in the US. Celia et al. (2011) and Postma et al. (2019) investigated CO_2 and brine leakage through abandoned wells using a stack of semi-analytical VE models that were connected by leakage through the abandoned wells. Bielicki et al. (2016) used the same semi-analytical multi-layered vertically-integrated modeling approach as Celia et al. (2011) to evaluate the monetary impact of CO_2 leakage on other subsurface activities, based on a 150 km × 150 km model of the Michigan basin.

The definition of a spatial scale for semi-analytical models is more difficult than for numerical models, as the semi-analytical models usually consider infinite lateral domains. Nonetheless, the models in Szulczewski et al. (2012) should be considered regional-scale models, as the domain of interest incorporates both the entire CO_2 plume and the entire pressure response; at the end of up-dip migration the CO_2 plume is likely larger than the envelope of the pressure response, as injection operation have ceased long before this time. On the other hand, the focus of the Celia et al. (2011) and Bielicki et al. (2016) studies is on the CO_2 plume and its immediate vicinity, and thus, those models should be considered to be a site-scale models although the abandoned wells are distributed over a large area (2500 km^2 and 22,500 km^2, respectively).

2.3. Vertically-integrated dynamic reconstruction multi-phase flow models

As noted above, the validity of the vertical equilibrium assumption is the main limitation for VE models. In order to extend vertically-integrated models beyond this limitation, Guo et al. (2014) developed a modeling approach that is based on the vertically-integrated multi-phase flow equations, but where a one-dimensional vertical fractional flow equation is solved to represent the vertical (non-equilibrium) flow dynamics of CO_2 and brine, instead of assuming instantaneous segregation as in the VE models. This approach is termed vertically-integrated dynamic reconstruction (DR) multi-phase flow approach. Other than the vertical fractional flow equation, the same set of equations is used as in VE models. Due to the additional complexity of vertical flow, DR models are solved numerically, both laterally and vertically, with one one-dimensional vertical model in each grid cell of the discretized vertically-integrated equations. The DR approach has also been extended to stacks of permeable formations (Guo et al.,

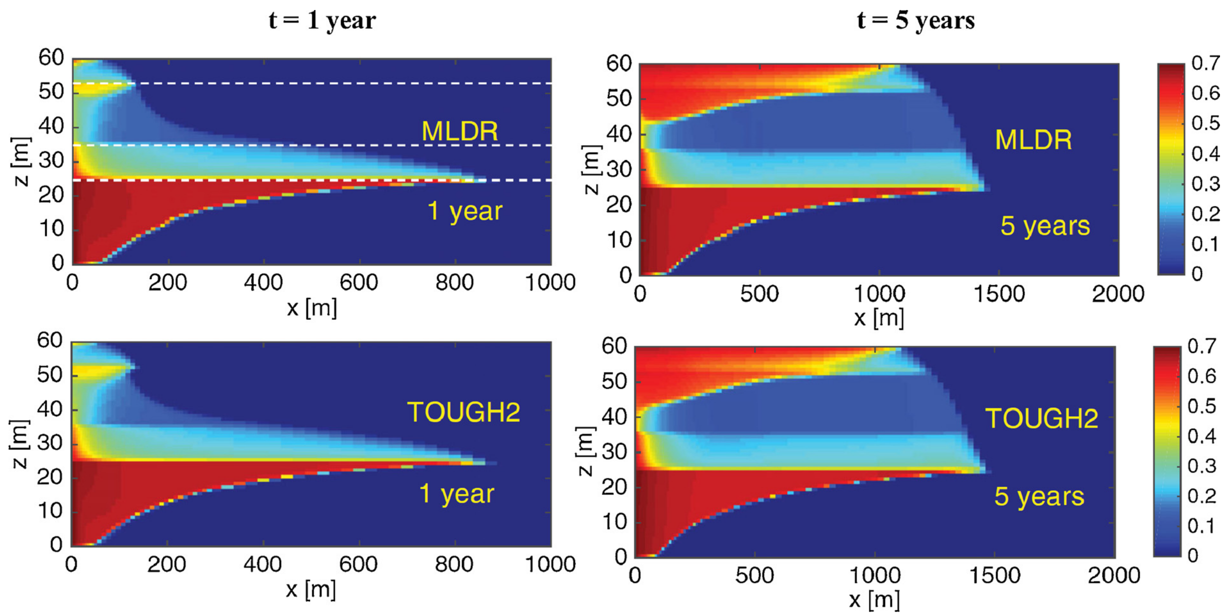

Fig. 7. Simulated CO_2 saturation cross-sections after 1 and 5 years of injection based on a 3D multi-phase flow model (TOUGH2) and a DR model (MLDR) for a hypothetical layered formation based on the Mt Simon Sandstone. Reproduced from Guo et al. (2016a) with permission from Wiley.

2016a), without the necessity of intervening low-permeability caprocks as in VE models.

DR models have not yet been applied to investigate GCS sites. However, comparisons of both single-layer and multi-layer DR models to three-dimensional multi-phase flow models show good agreement between the two approaches over a variety of formation parameters (Fig. 7), including parameters representative of the Mt Simon formation (Guo et al., 2014, 2016a). These test cases, all at the site scale, also show that the additional computational expense of solving the vertical fractional flow equation in each cell is small compared to the effort spent on solving the vertically-integrated equations, therefore not significantly reducing the computational efficiency of VE models (Guo et al., 2014). We note that though the DR models can capture the vertical two-phase flow dynamics, they are currently limited to either homogeneous or layered heterogeneous geological formations.

2.4. Three-dimensional multi-phase flow models

Three-dimensional multi-phase flow (3D multi-phase flow) models are based on three-dimensional mass balance (or for non-isothermal models the energy balance) equations for CO_2 and brine, along with three-dimensional Darcy's law flux equations, relationships linking capillary pressure to phase saturation and phase relative permeability, constitutive relationships for fluid properties, and the geometric constraint that the entire pore-space is occupied by the sum of the two phases. Deformation of the pore-space and changes in fluid densities due to pressure changes are presented by compressibility terms. The set of three-dimensional equations is then solved for the spatially-distributed – in all three spatial dimensions – primary unknowns: two phase pressures and two phase saturations.

3D multi-phase flow models are the most widely applied modeling approach for GCS simulation and, thus, have been applied at all three scales discussed here. For instance, Lindeberg et al. (2009) used a regional-scale (~25,000 m^2) 3D multi-phase flow model of the Utsira formation (Norway) to assess the dynamic storage capacity and to investigate the impact of active pressure management through brine production. Zhou et al. (2010) constructed a regional-scale (~240,000 km^2) 3D multi-phase flow model of the Illinois Basin (USA) to assess the potential for industrial-scale deployment of GCS in the basin (100 Mt/year for 50 years) and to determine the impact of GCS operations on up-dip freshwater resources. Michael et al. (2013) investigated the impact of hydrocarbon production induced underpressure on potential GCS operations in the Gippsland Basin (Australia) using a regional-scale (~45,000 km^2) 3D multi-phase flow model.

The applications of 3D multi-phase flow models at the site scale fall into three main categories: conceptual investigations, history matching of existing GCS sites, and project design of planned GCS operations. Conceptual investigations include studies of pressure management (Bergmo et al., 2011; Buscheck et al., 2012; Harp et al., 2017; Surdam et al., 2009), impact of model parameters (Court et al., 2012; Deng et al., 2016), enhanced CO_2 dissolution through brine circulation (Leonenko and Keith, 2008), impact of thermal effects (Dai et al., 2018; Oldenburg, 2007; Pruess, 2005), and automated optimization of GCS operations (Zhang and Agarwal, 2013). Example studies for history matching at existing sites are Kempka and Kühn (2013) adjusting permeabilities to match pressures at the injection well and monitoring wells (Fig. 8) and CO_2 arrival time at monitoring wells at the Ketzin site (Germany), Hosseini et al. (2013) matching pressures, saturation profiles and tracer arrival times at the Cranfield site (USA) through stochastic modeling, and Buscheck et al. (2016) matched the injection pressure at the Snøhvit site (Norway) by varying permeabilities of the reservoir and caprock and the location of sealing faults. Modeling studies by Flett et al. (2008) at the Gorgon site (Australia) and Senel and Chugunov (2012) at the ADM-Decatur site (USA) are examples for the use of 3D multi-phase flow models for project design.

Many of the well-scale applications of 3D multi-phase flow models are related to investigations of specific processes. For instance, several studies have used well-scale 3D multi-phase flow models to investigate enhanced dissolution of CO_2 into brine due to density-driven convective mixing (e.g., Elenius and Gasda, 2012; Emami-Meybodi et al., 2015; Ennis-King and Paterson, 2005; Ranganathan et al., 2012). Well-scale models have also been used to investigate flow in fractures (e.g., Raduha et al., 2016) and cemented wellbores (e.g., Jordan et al., 2015). Another example is modeling of mass transfer between fractures and the rock matrix in fractured reservoirs (March et al., 2018). Although CO_2 is expected to remain in its super-critical phase while in the injection formation, CO_2 may transition to the liquid or gaseous phase during vertical leakage (e.g., Pruess, 2011), requiring models to include three fluid phases.

Before we discuss modeling approaches that include the feedbacks

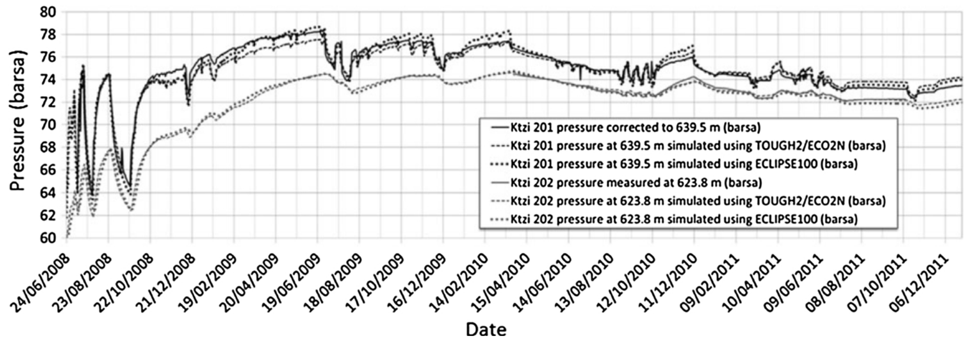

Fig. 8. Comparison of measured and simulated pressures in the injection well and a monitoring well at the Ketzin site using two 3D multi-phase flow models (TOUGH2/ECO2N and ECLIPSE100). Reprinted from Kempka and Kühn (2013).

from geochemistry and geomechanics on flow, it should be noted that 3D multi-phase flow models have been used to study geochemistry and geomechanics for cases without feedback. For instance, Doughty and Freifeld (2013) used a 3D multi-phase flow model as the basis for a reactive transport model to analyze a tracer study conducted at the Cranfield site (USA) and Morris et al. (2011) used the output from a 3D multi-phase flow model to calculate stresses to predict the surface uplift at the In Salah site (Algeria). In these cases, the 3D multi-phase flow model is run first for the entirety of the simulation duration and outputs (e.g., flow field, pressure response) are then used in separate geochemistry or geomechanical simulators.

2.5. Coupled flow, geomechanics, and geochemistry models

In fully coupled models, the impact of pore-space alteration through geomechanics and geochemistry is taken into account with feedback loops between flow and geomechanics and/or flow and geochemistry. Depending on the question being asked, the flow model is a numerical solution of either multi-phase (CO_2 and brine) or single phase (brine) flow equations. To include geomechanics, equations relating stresses to deformation (including rock failure) are added. Pore space alterations lead to changes in porosity and permeability, especially when existing fractures are opened or new fractures are created. The effects of geochemistry are represented by chemical constituent transport equations and chemical reaction equations. Impacts on flow occur through dissolution and precipitation of minerals in pores and through changes in fluid properties. Coupled models are either solved sequential, where flow, geochemistry and geomechanics are modeled separately, either by different modules within a simulator or by separate simulators, and information (e.g., pressure, porosity change) is shared between the modules/simulators at each time step, or simultaneously, where the governing equations for flow, geomechanics and geochemistry are solved together, so that information sharing occurs through direct coupling in the simultaneous solution of all equations within each time step. For sequentially coupled models with geochemistry, the geochemistry model is sometimes run with shorter time step size than the flow model to reduce the overall computational cost.

Coupled models often only focus on either geochemistry or geomechanics and the choice of process influences the model scale. Models including geomechanics are usually at the site scale, while models with geochemistry are often at the well scale. The most prominent case for geomechanics modeling related to GCS is the In Salah site (Algeria), due to the existence of fractures and measurable injection-induced surface uplift. For instance, Rinaldi and Rutqvist (2013) used a site-scale sequentially-coupled three-dimensional multi-phase flow model to explain the dual-lobe surface uplift patterns by including a fracture zone extending into the caprock (Fig. 9). The permeability of the fractures increased over the simulation time to represent creation of new fractures or opening of existing ones. Also based on the In Salah site, Preisig and Prevost (2011) used a simultaneously-coupled two-dimensional (vertical slice) multi-phase flow model to investigate the impact of thermal stresses (e.g., temperature difference between the formation and injected CO_2) on inducing or re-opening fractures. Coupled models have also been used to investigate induced seismicity from injection into basal aquifers (Zhang et al., 2013). A more detailed discussion on geomechanics relevant to GCS modeling can be found in Rutqvist (2012).

Flow models coupled with geochemistry have been used to investigate the impact of CO_2 injection on reservoir rock, the caprock and well cement. For instance, Audigane et al. (2007) found only little changes in porosity due to mineral precipitation/dissolution at the Sleipner site using a radially-symmetric two-dimensional multi-phase flow model coupled to a geochemistry model. In a study on changes in fracture aperture due chemical reactions Deng et al. (2016) coupled a single-phase flow (brine saturated with CO_2) model with geochemistry and found that mineral dissolution formed preferential flow paths. Brunet et al. (2016) investigated how initial fracture aperture and flow rate of CO_2-saturated brine through the fracture impact if a fracture in well cement will seal itself or grow, using a two-dimensional single-phase flow model coupled with geochemistry. Keating et al. (2013) used a two-dimensional flow model coupled with geochemistry to model deterioration of groundwater quality due to CO_2 leakage along faults.

2.6. Dual-domain models

In dual-domain models multi-phase flow in the fracture domain is solved the same as in unfractured systems, leading to a system of equations based on mass balance, Darcy's law and relationships between saturation, relative permeability and capillary pressure. The governing equations for the rock matrix blocks depends on their representation, ranging from relatively simple algebraic expressions for sugar cube models to an entire second set of multi-phase flow equations for dual-permeability models. The two sets of governing equations (one for the fracture domain and one for the rock matrix domain) are coupled through mass transfer functions modeling the mass exchange across the rock matrix-fracture interface.

March et al. (2018) applied a dual-domain model at the site scale to investigate the difference in CO_2 storage between a fractured and an unfractured hypothetical anticline. They used a 3D multi-phase model for the fractures and a sugar cube representation for the rock matrix, and found that the storage capacity of the anticline is lower for the fractured case, as the fracture domain has higher permeability, leading to an earlier arrival of CO_2 at the anticline spill points. This points to a time scale relevant to dual-domain modeling: if the migration in the fractures is fast relative to the rate of mass transfer between fractures and rock matrix, portions of the rock matrix may be bypassed for storage. A more detailed investigation into this time scale could potentially help determine conditions under which dual-domain models are necessary.

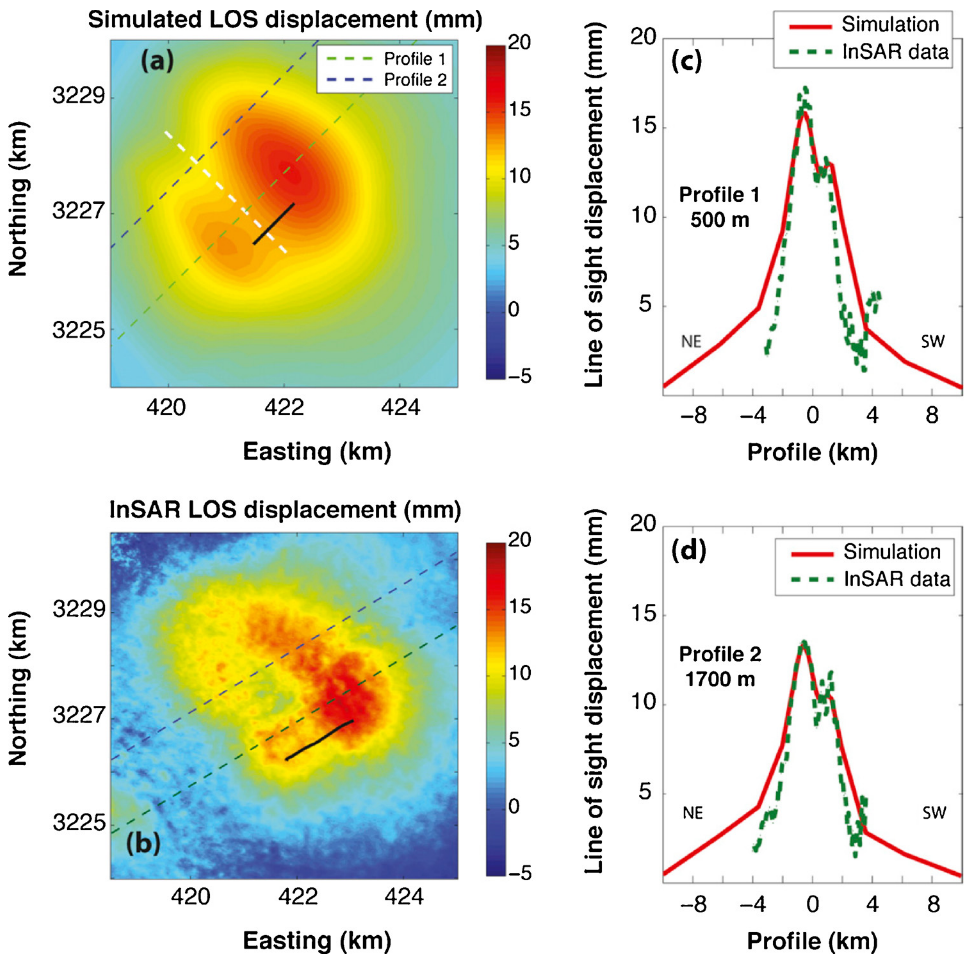

Fig. 9. Comparison of simulated and measured displacement at the In Salah site: (a) simulated displacement, (b) measured displacement, (c) displacement at profile 1, and (d) displacement at profile 2. Reprinted from Rinaldi and Rutqvist (2013) with permission from Elsevier.

Tao et al. (2019) developed a dual-domain model by combining a VE model for the fracture domain with a sugar cube model for the rock matrix domain. Based on a horizontal and homogeneous domain, they found that the VE dual-domain model compared well to a 3D dual-domain model, for cases with sufficiently high fracture permeability for the vertical-equilibrium assumption to be valid. Considering that fracture permeability can be expected to be high (e.g., Iding and Ringrose, 2010), these results also indicate, that CO_2 will likely accumulate in the upper parts of the fracture domain before significant mass transfer to the rock matrix occurs. Therefore, a sugar cube representation may be sufficient as there is no significant driver for vertical redistribution of CO_2 in the rock matrix. Again, more investigation is necessary to form a clearer understanding linking conditions to choices of rock matrix representation.

3. Choice of modeling approach guidelines

Based on the application of the different modeling approaches and the types of questions that need to be answered in the context of GCS, a set of guidelines for the choice of appropriate modeling approach is discussed in this section (see Table 1 for summary) to suggest questions and conditions where vertically-integrated approaches may be an effective and efficient option. It should be noted that when multiple different modeling approaches lead to the required level of accuracy the less complex one is chosen here, due to lower computational costs and data requirements.

3.1. Regional scale

Vertically-integrated single-phase models are the most appropriate choice for questions related to the regional-scale pressure response to GCS operations, as the pressure response outside of the CO_2 plume can be modeled by volume-equivalent brine injection. At the regional scale, the CO_2 plumes are small compared to the model domain, so that for most of the model domain the pressure is accurately modeled through single-phase flow. One example for investigations at the regional scale is lateral invasion of brine into updip freshwater zones of the injection formation (e.g., Nicot, 2008). Also, injection site selection in basins with ongoing or other planned GCS sites, where pressure interference between those sites could be studied with single-phase models (e.g., Huang et al., 2014). The relatively low computational costs make single-phase modeling amenable to Monte-Carlo type studies to investigate the impact of uncertain parameters – such as intrinsic permeability – on the pressure response. Due to the likelihood of significant spatial variability of parameters on the regional scale, a superposition of semi-analytical solutions to the single-phase equations does not lead to accurate modeling results, so that numerical solutions are generally necessary at the regional scale (Huang et al., 2014).

For some regional-scale questions the location of CO_2 plumes is an important consideration, and thus, multi-phase flow models are needed. Studies of the deployment of multiple GCS operations in a basin is an example where the locations of the CO_2 plumes can be important. The location of CO_2 plumes is important to investigate the intersection of CO_2 plumes from neighboring injection sites (Bandilla et al., 2012; Person et al., 2010; Zhou et al., 2010), the containment of CO_2 in a

Table 1
Overview of modeling approach guidelines.

Question	Scale	Suggested approach	Example
Updip displacement of brine – freshwater interface	Regional	Vertically-integrated single-phase	Nicot (2008)
Pressure interference from different injection operations	Regional	Vertically-integrated single-phase	Huang et al. (2014)
Dynamic capacity estimate	Regional and site	Vertically-integrated multi-phase	Bandilla et al. (2015)
CCS deployment scenarios	Regional	Vertically-integrated multi-phase	Bandilla and Celia (2017)
Long term updip migration of CO_2	Regional	Vertically-integrated multi-phase (semi-analytical and numerical)	Szulczewski et al. (2012)
History matching	Site	3D multi-phase or vertically-integrated multi-phase[a]	Kempka and Kühn (2013)
Operational design	Site	3D multi-phase, vertical equilibrium multi-phase, or dynamic reconstruction multi-phase (depending on injection and formation parameters)[a]	Flett et al. (2008)
Trapping mechanisms	Site	3D multi-phase coupled with geochemistry	Zhang et al. (2016a)
Leakage along concentrated pathways	Site or regional	Vertically-integrated multi-phase (semi-analytical and numerical)	Celia et al. (2011)
Process investigation	Well	3D multi-phase potentially coupled with geochemistry and geomechanics	Ennis-King and Paterson (2005)

[a] Model choice may vary over the life of a project as more datasets become available.

specific area (Deng et al., 2012), or the placement of production wells for active pressure management (Bandilla and Celia, 2017) and protection of sensitive areas (e.g., fault zone with risk of vertical CO_2 leakage) (Cihan et al., 2015). Another example where CO_2 migration is important at the regional scale are studies of long-term updip CO_2 migration (Szulczewski et al., 2012). VE models are the most appropriate choice for modeling multi-phase flow at the regional scale, because the injection formation is thin relative to the lateral extent of the CO_2 plume, so that the vertical equilibrium assumption is likely to be valid. Therefore, VE models are expected to give accurate modeling results at much lower computational costs than 3D multi-phase flow models. For most cases the VE governing equations need to be solved numerically as formation properties are expected to vary at regional scales. While VE models are often restricted to multi-phase flow modeling, additional processes can be added. For instance, dissolution and constituent transport can be added for storage safety modeling (Gasda et al., 2011), as well as thermal effects (Andersen and Nilsen, 2018; Gasda et al., 2004).

The estimation of storage capacity is another topic that is usually addressed at the regional scale. Static estimation approaches are based on the available pore space reduced by a set of storage efficiency factors, and thus need no modeling. Dynamic estimation approaches take into account the injection-induced pressure increase and the distribution of CO_2 in the domain, and therefore require multi-phase flow modeling (Bandilla et al., 2012; Person et al., 2010; Ricard et al., 2016; Zhou et al., 2010). VE models are the most appropriate choice here, for the same reasons as discussed in the previous paragraph. Also, capacity estimates are often conducted with relatively scarce data, so that the spatial distribution of rock properties is not well known. In such cases, it may be reasonable to assume constant rock properties, which allows for the use of semi-analytical solutions to the VE governing equations. Due to their high computational efficiency the semi-analytical models can be used in Monte Carlo-type studies to investigate the uncertainty in storage capacity from uncertainty of rock properties. Semi-analytical VE models are also the most appropriate approach for capacity estimates based on long-term balance of updip CO_2 migration, dissolution and residual trapping, as models for such studies extend over large spatial scales to cover the migration from injection to outcrop and migration may take hundreds of years (Szulczewski et al., 2012); the computational effort required by more complex modeling approaches would make such studies infeasible.

3.2. Site scale

Calibrating models to measured observations – often termed history matching – is an important tool to better understand the subsurface flow system and thus leads to more accurate predictions. History matching occurs at the site scale with pressure at the injection well or off-set wells and CO_2 breakthrough at off-set wells serving as observations. History matching has been conducted using site-scale 3D multi-phase flow models in order to capture heterogeneous domains (e.g., Buscheck et al., 2016; Hosseini et al., 2013; Kempka and Kühn, 2013). However, if lateral heterogeneity has a stronger impact than vertical heterogeneity, VE models can also be applied to history matching (e.g., Bandilla et al., 2014; Nilsen et al., 2011). Recent advances in VE modeling, such as inclusion of vertical heterogeneity of rock parameters (Bandilla et al., 2017) and non-equilibrium brine drainage (Becker et al., 2017), are extending the capabilities of VE models to more heterogeneous domains, therefore extending their potential for history matching at the site scale. VE models are especially attractive in conjunction with automated calibration tools, due to VE models' computational efficiency. History matching may also be conducted based on sampling brine constituents at monitoring wells or deformation of the subsurface resulting in surface uplift. If geochemistry or geomechanics have an impact on flow, models directly coupling flow and the other processes are required (e.g., Rinaldi and Rutqvist, 2013), otherwise geochemistry and geomechanics can be treated as a post-processing step (e.g., Doughty and Freifeld, 2013; Morris et al., 2011). It should be noted that while incorporating more observations in the history matching process is generally better, adding additional processes – with additional uncertain parameters – can make it more difficult to determine a unique parameter set for a model.

Understanding the flow system at a GCS site is usually an iterative process, with very little data during the initial stages, especially when injecting into a hitherto unused formation (i.e., no prior oil and gas production). As a GCS project continues, more data about the injection formation become available through core plugs from drilling injection and monitoring wells, well testing and, later, pressure and other monitoring data during the CO_2 injection. With the increase of available data the understanding of the flow system becomes more refined, so that the most appropriate modeling approach may change over the course of a GCS project. Initially, there may not be enough data to support more than a site conceptualization consisting of a single homogeneous layer, in which case a semi-analytical VE model is most appropriate to conduct preliminary investigations. A more complex model is chosen once the current model is no longer able to fit the data, potentially leading all the way to coupled flow and geochemistry/geomechanical models.

The main difference between VE and 3D models is that transient vertical flow within a formation is not accounted for in VE models. Transient vertical flow is usually important close to the injection well, for formations with low intrinsic permeability, partially-penetrating injection wells (e.g., horizontal wells), or heterogeneity in the vertical direction that acts as discontinuous baffles. DR models are designed to represent transient vertical flow and therefore could replace 3D multi-phase flow models at the site scale. While initial results from DR modeling at the site scale show promising results (Guo et al., 2016a), more testing of the applicability of the DR modeling approach is necessary, especially for cases with discontinuous horizontal layers. Therefore, 3D multi-phase flow models are the appropriate choice at the site scale, if transient vertical flow is important. DR models are probably not applicable at the regional scale, as transient vertical flow becomes less important for larger domains.

Questions related to specific injection sites (e.g., maximum allowable injection rates, history matching, storage capacity) are usually addressed at the site scale (e.g., Flett et al., 2008; Senel and Chugunov, 2012). VE, DR and 3D multi-phase flow models are appropriate modeling choice here, as heterogeneity can be expected to play a significant role at the site scale. For formations with vertical intrinsic permeability of less than ~100 mD the vertical equilibrium assumption is less likely to be valid, so that DR models are the more appropriate choice (Guo et al., 2014). The ~100 mD threshold is based on common formation and injection parameters; the threshold is expected to be lower for thinner formations and for conditions with a higher density difference between brine and CO_2. 3D multi-phase flow models become the appropriate choice when heterogeneity in intrinsic permeability, such as discontinuous horizontal baffles, leads to significant complexity in vertical flow paths (Deng et al., 2012). While DR models have been shown to accurately simulate formations with layered heterogeneity patterns – as often found in sedimentary formations – their performance for more unstructured heterogeneity patterns still needs to be investigated (Guo et al., 2016a). If the impact of geochemistry or geomechanics requires coupled models, either 3D multi-phase flow or VE models may be used as the flow component, with the choice of flow model based on the guidelines mentioned earlier in this paragraph. However, coupled simulators using 3D multi-phase flow models are well established, while coupled simulators based on VE flow model are still being developed.

Studies of storage safety often are interested in the form in which CO_2 is present: mobile pure-phase CO_2, pure-phase CO_2 trapped by capillary forces, CO_2 dissolved in brine or mineralized CO_2. Capillary trapping and dissolution (including the impact of density driven convective mixing) have been implemented in VE (Gasda et al., 2011) and 3D multi-phase flow models (Baz et al., 2016), so that the choice of modeling approach should be guided by the criteria discussed above, just as for models not focusing on capillary trapping and dissolution. To the authors' knowledge precipitation and dissolution of carbon-based minerals has only been implemented with models coupling 3D multi-phase flow with geochemistry, although there do not appear to be theoretical issues in coupling geochemistry with VE flow models. While carbon mineralization has often been neglected due to the long timescales involved, recent studies of GCS in basalts show mineralization becoming significant on the order of years or less (Matter et al., 2016). Developing geochemistry models coupled with VE flow models, therefore becomes a relevant research topic.

Some GCS questions require inclusion of geochemistry and geomechanics at the site scale. If there are no feedbacks from the additional processes to flow (e.g., tracer studies, surface uplift), the flow model can be chosen independently from the process models, as the models can be run sequentially (e.g., Doughty and Freifeld, 2013; Morris et al., 2011). In this case the modeling approach for flow should be chosen based on the guidelines presented above. However, it may be necessary to have the same grid for the flow model and the process models, in which case 3D multi-phase flow models are the most appropriate case. For cases where feedbacks between flow and other processes are important (e.g., changes in porosity due to precipitation/dissolution, fracture reactivation) coupled models are required. Currently, almost all coupled models rely on 3D multi-phase flow models for the flow component (e.g., Audigane et al., 2007; Rinaldi and Rutqvist, 2013). So, while other flow modeling approaches may be more appropriate based on the spatial scale of a specific model, the model choice is restricted to the 3D multi-phase flow approach for coupled models. However, coupled models based on VE flow models are in development (Bjørnarå et al., 2016).

CO_2 and brine migration along concentrated leakage pathways is also important to determine storage safety. The difference in spatial scales between the leakage pathways (on the order of tens of centimeters to tens of meters) and the storage formation (hundreds of meters to hundreds of kilometers) makes flow modeling difficult, as the areas around the leakage pathways need to be finely resolved, leading to very high computational demand. The scale difference is especially high if the leakage pathways are abandoned wells. In this case, an additional complicating factor is that the permeabilities and locations of the abandoned wells are often unknown, and therefore Monte Carlo-type approaches – with a need for multiple model realizations – are often necessary to determine leakage risk. VE models are the appropriate modeling approach for such leakage studies, because these studies tend to have large spatial extents and the computational efficiency of VE models reduces the computational effort. Semi-analytical vertically-integrated multi-phase flow models should also be considered, due to their high computational efficiency; especially in cases where data availability in the storage formation is too low to justify detailed geological models (Celia et al., 2011). For cases of brine leakage along concentrated pathways (i.e., pathways located outside of the CO_2 plume) single-phase models are the most appropriate choice. Semi-analytic vertically-integrated models are applicable for simple geometries (Cihan et al., 2013), but 3D single-phase models are required for more complex geometries and/or changing salinity (Kissinger et al., 2017).

3.3. Well scale

Models at the well scale and below are sometimes used to study particular processes, instead of GCS itself, often with the goal to upscale the impact of that process for use in models with spatial extent more relevant for GCS modeling. The study of dissolution of CO_2 into brine, with resulting gravity enhanced mixing is one example (e.g., Elenius and Gasda, 2012; Emami-Meybodi et al., 2015; Ennis-King and Paterson, 2005; Ranganathan et al., 2012). Models at the well scale are also used to study wellbore leakage risks using 3D multi-phase flow models in combination with Monte-Carlo approaches (e.g., Jordan et al., 2015). Also, these types of studies often need to include additional processes (e.g., geochemistry for dissolution studies) and coupling of 3D flow models with other processes models is well established. 3D multi-phase flow models are the most appropriate choice here, due to the potential importance of vertical flow and the coupling to other processes models.

4. Conclusions

Computational modeling of CO_2 and brine migration is an essential tool for investigating questions related to GCS. However, there are many different modeling approaches that can be applied to GCS modelling. The modeling approaches discussed here range from single-phase models to investigate the large-scale pressure response to CO_2 injection, to modeling approaches that couple multi-phase flow to other processes such as geochemistry and geomechanics. The modeling approaches may also differ in their representation of the flow domain. While a three-dimensional representation allows for the greatest flexibility of flow patterns, vertically-integrated two-dimensional approaches have the advantage of higher computational efficiency.

While several modeling approaches may be applicable to answer a specific GCS related question, the guidelines presented here aim at choosing the least complex modeling approach that gives reliable results. For instance, a three-dimensional multi-phase flow model could be used to determine the interaction of pressure responses of multiple

GCS sites accessing the same formation, but a vertically-integrated single-phase model would lead to the same results, with lower data requirements and computational effort, and is therefore deemed a more appropriate choice here. It should be noted, that the most appropriate modeling choice may change over the lifetime of a GCS operation, as more data become available (e.g., injection well cores, pressure response to injection in off-set wells) and the pertinent questions change (e.g., storage capacity, injection rate scheduling). Three spatial scales are defined to help guide the modeling approach choice: well scale (immediate vicinity to the wellbore; tens of centimeters to several meters), site scale (area containing the CO_2 plume of a single site and its vicinity; hundreds of meters to tens of kilometers) and regional scale (area that contains majority of pressure response; tens to hundreds of kilometers).

Based on questions relevant to GCS and the three spatial scales the following guidelines can be formulated (see Table 1 for summary). Vertically-integrated single-phase models are the appropriate choice for questions related to the pressure response outside of the CO_2 plume at both the site and regional scales. Vertically-integrated multi-phase models are the appropriate choice at the regional scale if the locations of the CO_2 plumes are important along with the pressure response (e.g., dynamic capacity estimates, active pressure management). At the site scale vertically-integrated multi-phase flow models are the appropriate choice, if the vertical segregation of CO_2 and brine is fast (often the case for intrinsic permeabilities above 100 mD for usual GCS conditions). Vertically-integrated dynamic reconstruction models are the appropriate choice at the site scale, if vertical segregation is not at equilibrium and there is no other significant vertical flow. Also, any significant horizontal layering needs to be continuous. Three-dimensional multi-phase flow models are the appropriate choice at the site scale for cases with complex vertical flow patterns. At the well scale three-dimensional multi-phase flow models are the appropriate choice, due to the importance of vertical dynamics at such small scales. Some GCS related questions require that other processes, such as geochemistry and geomechanics, are coupled with multi-phase flow models (e.g., surface uplift, mineral dissolution). If there is no feedback from these processes to flow, then the flow model should be chosen based on the guidelines mentioned above, as including the other processes can be seen as a post-processing step. For cases with feedbacks between flow and the other processes (e.g., changes in porosity through mineral dissolution) three-dimensional multi-phase flow models are the appropriate choice, mainly because the other processes are usually modeled on three-dimensional grids as well. However, the recent development of a vertically-integrated approach for geomechanics points to the potential for coupled vertically-integrated models in the future.

The guidelines presented here are based on the least complex approach that can answer a specific question with sufficient accuracy, but there are many other factors that guide a user in the choice of a modeling approach. For instance, a user will tend to choose a modeling approach (or even a specific modelling software) they are familiar with as they are confident in the results and learning a new approach may take significant time. The "popularity" of the modeling approach is also an important factor, as the results are more likely to be accepted by stakeholders and widespread use of a modeling tool often comes with existing pre- and post-processing tools. Keeping these other factors in mind, we hope this article helps modelers to consider alternative modeling approaches when embarking on new projects.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgments

This material is based upon work supported by the Carbon Mitigation Initiative at Princeton University and by the U.S. Department of Energy (DOE) National Energy Technology Laboratory (NETL) under Grant Number FE009563. This project is managed and administered by Princeton University and funded by DOE/NETL and cost-sharing partners. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

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