Modeling Changes in Pressure due to Migration of Fluids into the Above Zone Monitoring Interval of a Geologic Carbon Storage Site

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ABSTRACT

An increasing emphasis on the industrial-scale implementation of Carbon dioxide (CO₂) storage in geological formations has led to the development of whole-system models to evaluate performance of candidate geologic storage sites and the environmental risk associated with them. Components of that engineered geologic system include the storage reservoir, overlying aquitards (primary caprock and secondary seals) and aquifers (including the above zone monitoring interval, or AZMI, directly overlying the primary seal), and potential leakage pathways including wells, fractures, and faults. Leakage of CO₂ and brine through the primary seal to the overlying porous and permeable formations (AZMI) may occur due to the seal's intrinsic permeability and/or the presence of natural fractures or induced perforations or fractures in the caprock. AZMI monitoring may provide a potentially useful source of information about seal performance and subsurface pressure response to potential CO₂ and/or brine leakage from the reservoir. Unfortunately, full complexity simulations of the geologic storage system are not computationally affordable, especially given the need to develop many realizations to

32 evaluate uncertainties in system performance. Thus, the goal of the current work is to
33 present a novel reduced order model (ROM) for AZMI that simulates fluid (i.e., CO₂ and
34 brine) flow above the seal, and verify performance of the ROM. The AZMI model
35 predicts spatial changes in pressure over time in the zone above the primary seal due to
36 migration of fluids from the reservoir. A case is examined wherein CO₂ is injected into a
37 storage reservoir for 30 years and a heterogeneous primary seal exists above the reservoir
38 with some permeable zones. The model results are verified against those of a numerical
39 simulator. The new AZMI model provides an improvement in computation time by a
40 factor of approximately 2000 times to that of the numerical simulator and provides
41 predictions that approximate those of the comparable numerical simulation.

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43 **Keywords:** Geologic CO₂ Storage, CCS, Reduced Order Modeling, Risk Assessment,
44 Monitoring, Reservoir Simulations.

1. INTRODUCTION

Significant changes in average temperature around the globe over the past century have raised concerns for humankind and the stability of earth's ecosystem. Projections of recent emission trends assuming a business-as-usual scenario suggest that potential temperature increases between 1.1–6.3°C by the end of the 21st century (Bachu, 2008; IPCC, 2013). Increases in the atmospheric concentration of carbon dioxide (CO₂) and other greenhouse gases (GHGs) are considered one of the major causes of global warming (IPCC, 2013). An International Energy Agency (IEA) study indicates that CO₂ emissions will increase by 130% by 2050 in the absence of new policies or supply constraints because of increased fossil fuel usage (IEA, 2008, 2013). Addressing climate change through the reduction of anthropogenic greenhouse gas emissions is one of the most significant challenges of our time.

CO₂ capture and storage (CCS) is one of a portfolio of solutions for the reduction of anthropogenic greenhouse gas emissions to the atmosphere. This process involves separating CO₂ from the gaseous process stream of large industrial emitters, compressing the separated CO₂ to form a liquid phase, transporting the CO₂ via pipeline to an injection site, and injecting the captured CO₂ into deep geologic formations. Specifically, underground formations such as depleted oil and gas reservoirs and deep saline formations are two of the targets most commonly considered for the subsurface storage of CO₂ (IPCC, 2005). However, there are outstanding regulatory, market, and environmental hurdles to overcome before CCS can be widely deployed at a commercial scale.

The increasing emphasis on the commercialization and full-scale implementation of CCS has led to the development of system-wide mathematical models for the quantitative assessment of performance potential geologic storage sites and associated risks. The United States Department of Energy (DOE), through its National Risk Assessment Partnership (NRAP) Program (NETL, 2011), has developed methodologies, system component models, and integrated assessment models (IAMs) for application in evaluating risk performance of geologic storage systems (Pawar et al., 2016). The IAMs

are system models that couple predictive models of the primary sub-system components of the storage system (i.e., storage reservoir, caprock seal, migration pathways including wellbores, faults and fractures, groundwater aquifers, and the atmosphere), with the goal of ensuring long-term storage security and environmental risk performance in the context of system uncertainty. NRAP quantitative assessments consider midpoint indicators of risk, including potential impairment of underground sources of drinking water, and potential leakage of CO₂ to the atmosphere. The integration of fully complexity models of individual system components in an IAM framework would result a model that is computationally expensive – taking potentially hundreds of hours to run a single realization of the system model. To address this limitation, NRAP has employed the approach of constructing computationally efficient reduced order models (ROMs) - based on results from numerical models – and incorporating those ROMs into the IAM framework. In general, ROM is a technique for reducing the computational complexity of mathematical models in numerical simulations. Several types of ROMs can be developed, including simple correlations, look-up tables, analytical expressions, simple regressions, reduced physics models, and surrogate models (Zhang and Pau, 2012; Bromhal et al., 2014; Soeder et al., 2014). In all cases, the ROMs represent abstractions, when appropriate, and are based on detailed physical and chemical descriptions of the key subsystems at the sites (Pawar et al., 2013). This study presents a novel ROM developed to predict pressure changes due to migration of fluids into the above zone monitoring interval (AZMI), which is an important component of the IAM. A flux aggregation approach developed by the authors is applied in the ROM to significantly reduce the running time of the model without compromising the accuracy of the model. Details of the flux aggregation approach can be found in section 2.4.

In its simplest conception, a geologic storage system can be considered to be made up of three components: (1) the porous/permeable storage reservoir formation where the CO₂ is injected and stored; (2) a relatively impervious rock layer designated as the seal or caprock, which overlays the reservoir; and (3) a heterogeneous geologic zone, which extends from above the caprock to the deepest underground source of drinking water. The caprock overlying the reservoir has an intrinsic permeability through which CO₂ may

leak; in a good candidate storage site, that intrinsic caprock permeability will be quite low. These sealing layers may also contain natural faults or fractures and other leakage pathways (e.g., legacy wells), all of which may represent potential conduits for the vertical migration of injected CO₂ and connate brine to overlying formations and potentially to overlying receptors of concern. To verify storage permanence and understand the extent of potential unwanted fluid migration in the subsurface, it is important to design approaches to effectively and efficiently monitor the performance of these engineering systems. One way to detect such leakage is the use of atmospheric or near-surface monitoring technologies; however, these techniques may not identify leaks until after receptors of concern have been impacted. It may be useful to couple near-surface measurement to verify that those receptors of concern are not endangered, with direct or indirect deep subsurface monitoring techniques to detect potential unwanted condition near the storage reservoir. Ideally, these deep monitoring techniques will have the capability to identify and resolve the onset, location, and volume of leakage from the reservoir in a systematic and timely manner. The monitoring of pressure changes, as an indication of leakage, represents one such approach (Sun et al., 2012; Jung et al., 2013; Azzolina et al., 2014; Wang and Small; 2015). Recent studies (Nicot et al., 2009; Hovorka et al., 2013) show the potential utility of monitoring to detect and estimate leakage and pressure changes above the caprock.

There have been numerous studies about numerical simulation of geologic CO₂ storage (e.g., Oldenburg et al., 2001; Nordbotten et al., 2004; Pruess, 2004; Xu et al., 2004; Bielinski, 2007; Bryant et al., 2008; Jiang, 2011; Pruess and Nordbotten, 2011; Cihan et al., 2012, Vilarassa et al., 2013; Heath et al., 2014). These models range from simplified analytical approaches to three-dimensional (3D) multi-phase and multi-component models. U.S. DOE (2009) provides an extensive list of 20 numerical codes that have been applied to understand the geologic CO₂ storage performance. Numerical models that couple physics, chemistry, and/or geomechanics can generate high quality, technically credible and defensible results. These models are, however, computationally expensive, often requiring tens of hours to calculate a single realization; this limits their utility for rapid scenario evaluation, sensitivity analysis, and uncertainty quantification, which

could call for calculation of hundreds or thousands of realizations. The aim of this study is to develop a ROM to simulate the pressure and CO₂ saturation response over time in the geologic interval directly above the primary seal of the geologic storage confining system, termed the above zone monitoring interval (AZMI), which results from fluid migration from the storage reservoir. The construction of a computationally efficient ROM for the AZMI is useful addition to an IAM for CO₂ storage because it allows consideration of the AZMI response to potential CO₂ leakage from the storage interval, and exploration of how that signal can be used for deep subsurface monitoring and early detection of unexpected seal performance. A generalized schematic of the IAM framework into which the AZMI ROM will be integrated is shown in Figure 1. The figure outlines the hierarchy of sub-system level ROMs as they reside within a proposed IAM framework, and how information is passed between them. Stated simply, in that hypothetical IAM framework the results from storage reservoir ROM (pressure and saturation at the reservoir/seal interface) are passed on to the primary seal ROM which then passes the information to the AZMI ROM, and so on, capturing important fluid flow and pressure response through the system. In the present study, development of a ROM that predicts changes in pressure in the AZMI due to fluid leakage from the reservoir and CO₂ flow through brine saturated geologic formations is targeted. This manuscript provides a description of the AZMI model formulation (Section 2), discusses a baseline case study of its application (Section 3), and summarizes the case study results and the verification of the ROM performance based on comparison with comparable results from a detailed numerical model - TOUGH2 (Pruess, 2005).

2. ABOVE ZONE MONITORING INTERVAL (AZMI) ROM

As described in the previous section, the AZMI is the porous and permeable geologic interval directly above the primary seal of the geologic storage confining system, i.e., the aquifer immediately overlying the impermeable caprock layer. The AZMI ROM divides the model domain into 10,000 uniformly sized grid blocks (100 by 100 gridblock array), with the dimensions of each grid block dictated by the size of the domain required to represent site-scale geologic storage. The 100 by 100 grid system is selected to match

that prescribed for reservoir resolution in NRAP's IAM (for potential integration at a later stage), though the AZMI ROM is designed as a stand-alone ROM. As can be seen from the hypothetical systems level hierarchy (Figure 1), the flux output from the seal is the primary input for the AZMI model, which it receives for each time step. In the present study, we use CO₂ and brine flux as input. TOUGH2 is used to create these flux inputs from the seal. However, the AZMI model can accept input from any seal model as long as those inputs are consistent with the AZMI modeling structure.

2.1. AZMI ROM Assumptions

There are certain theoretical assumptions that underlie the AZMI ROM. The AZMI model assumes that the subsurface layer of interest is situated at a sufficient depth to ensure that free CO₂ remains in the supercritical state (i.e., depth of the AZMI is at a depth of ~735 m or greater). In addition, it is assumed that the AZMI is initially saturated with brine, with open lateral and vertical boundaries. For computational purposes, only vertical upward flow is considered for the flux and geomechanical impacts on the AZMI response are neglected. Flow is also considered to be laminar, permitting the application of Darcy's law. It is assumed that the flux entering the AZMI from the caprock seal is comprised of two phases, namely CO₂ and formation brine (Nordbotten and Celia, 2006; Lindner, 2015). The impact of CO₂ dissolution in brine within the AZMI has been ignored. In this system, CO₂ is considered to be the non-wetting fluid and brine is considered to be the wetting fluid.

2.2. Governing Equations for Two-Phase Flow

The AZMI ROM predicts changes in pressure and CO₂ saturation responses over time and space within the AZMI. This predictive capability provides an assessment of to what extent migration of fluids from the reservoir results in cases of heterogeneous caprock permeability. It also helps in understanding the subsurface response, and implications of that response, for diagnostic purposes of seal integrity, plume disposition, pressure based

monitoring and related uncertainties. The ROM is also able to predict the gas saturations above the AZMI.

The widely-employed mass and momentum conservation equations are used to describe two-phase flow in the AZMI. As part of the momentum balance, Darcy's law is extended to multi-phase flow using the additional constraint:

$$S_{brine} + S_{CO_2} = 1$$

For laminar flow, Darcy's law for fluid α (under the assumption of negligible capillary pressure) is expressed as:

$$\mathbf{q}_\alpha = -\frac{k k_{r\alpha}}{\mu_\alpha} \nabla (p - \rho_\alpha g z) \quad (2)$$

where, $\mathbf{q}_\alpha$ is the Darcy flux in α phase [LT^{-1}], k is the intrinsic permeability [L^2], $k_{r\alpha}$ is the relative permeability of the α phase [$-$], μ_α is the viscosity of the α phase [$ML^{-1}T^{-1}$], ∇ is the differential operator given by divergence of gradient of a parameter, p is the pressure, ρ_α is the fluid density in the α phase [ML^{-3}], g is the gravitational acceleration constant, and z is the vertical coordinate [L].

The mass conservation equation for CO_2 and brine is then expressed as:

$$\frac{\partial}{\partial t} \phi \rho_\alpha S_\alpha + \nabla \cdot \mathbf{q}_\alpha = 0 \quad (3)$$

where, ϕ is the porosity [$-$], S_α denotes the α phase saturation [$-$] and t is the time of flow [T].

The relative permeability of phase α is defined as the ratio of permeability of α phase (k_α) to that of the intrinsic permeability:

$$k_{r\alpha} = \frac{k_\alpha}{k} \quad (4)$$

2.3. Closure Relations

Relative permeability has important implications for fluid flow in subsurface geological systems. The two most widely used models developed to formulate relative permeability are the Brooks-Corey (Saadatpoor et al., 2010; Krevor et al., 2012) and van Genuchten (Lucier et al., 2006; Bielinski, 2007) models. In this study, the Brooks-Corey Model is used to define relative permeability in the AZMI ROM.

According to Brooks and Corey (1966), the relative permeability for brine ($k_{r,brine}$) and CO_2 (k_{r,CO_2}) can be represented as:

$$\begin{aligned} k_{r,brine} &= S_e^{\left[\frac{2+3\beta}{\beta}\right]} \\ k_{r,CO_2} &= 1 - S_e^2 [1 - S_e^{2+3\beta}] \end{aligned} \quad (5)$$

where the Brooks-Corey parameter β is related to the distribution of pore sizes and the effective saturation (S_e) is defined as the normalized wetting phase saturation adjusted to define two-phase flow in the different zones of interest (Luckner et al., 1989; Lindner, 2015). In the case of low wetting phase saturations, there exists a zone where the flow of the wetting phase does not remain coherent and is defined as the residual wetting phase (the brine in this study) saturation. Similarly, at high wetting phase saturations, there exists a zone where the flow of the non-wetting phase (the CO_2 in this study) does not remain coherent and is defined as residual non-wetting phase saturations. Since both CO_2 and brine exhibit coherent flow, the effective saturation is defined in the AZMI ROM as:

$$S_e = \begin{cases} \left(\frac{S_{brine} - S_{r,brine}}{1 - S_{r,brine} - S_{r,CO_2}} \right), & \text{if } S_{r,brine} < S_{brine} < (1 - S_{r,CO_2}) \\ 0, & \text{if } S_{brine} \leq S_{r,brine} \\ 1, & \text{if } S_{brine} \geq (1 - S_{r,CO_2}) \end{cases} \quad (7)$$

When two immiscible phases exist within the same pore space, there is an interfacial tension between the two phases that results in a pressure differential, which must be overcome to initiate flow. The pressure differential between the two phases (i.e., wetting and non-wetting phase) is called the capillary pressure (P_c). Capillary pressure highly influences the flow processes and can also prevent the upward migration of CO₂ in geologic storage formations (Chalbaud et al., 2010; Nielsen et al., 2012; Lindner, 2015).

With CO₂ and brine as the two phases, capillary pressure is defined as:

$$P_c = P_{CO_2} - P_{brine} \quad (8)$$

The experimental findings of Brooks and Corey established that capillary pressure could be related to effective saturation using a power law:

$$P_c = \left[\frac{P_b}{(S_e)^{\frac{1}{\beta}}} \right], \text{ if } 0 < S_e \leq 1$$

where, P_b is a material constant, termed as the bubbling pressure. This constant is essentially a curve fitting parameter for the Brooks and Corey relative permeability model. The bubbling pressure is understood as the capillary pressure at 100% effective saturation from the empirical Brooks and Corey relative permeability curve.

2.4. k-means Clustering

As described previously, the AZMI model is constructed to accommodate 100 by 100 grid blocks, receiving flux input from the seal model for each of the individual blocks. Rather than manage each of these fluxes individually, which can become computationally expensive, a flux aggregation approach using k-means spatial clustering is used to describe the CO₂ and brine fluxes of the entire space. The following section explains the pressure response calculation performed using this approach.

To increase the computational efficiency of the AZMI ROM, the system space is aggregated into a few clusters with similar properties/features (we use the seal property, permeability). The spatial clustering is based on a widely-accepted cluster analysis methodology in data mining known as k-means clustering (MacQueen, 1967). The concept of k-means clustering aims to partition a given set of n data, $\{x^{(1)}, x^{(2)}, \dots, x^{(n)}\}$, into a few “cohesive” k clusters in which each data point belongs to the cluster with the nearest mean, serving as a prototype of the cluster.

A flux-based aggregation approach, in which the fluid flux coming from the seal in each grid block present in the individual clusters is used to compute the total CO₂ and brine flow in each of these clusters, is developed by the authors. The total incoming flux is assumed to enter the AZMI from the centroid of the individual clusters. Mathematically, total incoming volumetric flux flow of the α – phase for the j^{th} cluster (among “ k ” number of clusters) containing “ m ” number of grid blocks can be represented as:

$$Q_{\alpha}^j = \sum_{i=1}^m q_{\alpha_i}^j \quad (10)$$

where, q_{α_i} is the flux flow in the α phase for the i^{th} cell.

In the current model, for a set of 10,000 data points (each grid in the 100 by 100 grid block system represent a data point), five clusters have been used for the simulations since the seal permeability has five high permeable regions. The user can also use the model for different sets of clusters as intended. With greater the number of clusters, the prediction will more accurately match that of the detailed numerical simulation, but the computational time will also increase with increase in number of defined clusters.

2.5. Analytical Solution

The AZMI ROM uses the analytical solution for CO₂ plume movement in the storage formation derived by Nordbotten et al. (2005) to quantify pressure changes in the zone

overlying the caprock due to the leakage of CO₂ through the caprock. The CO₂ flow in a brine-saturated formation solution by Nordbotten and colleagues (Nordbotten et al., 2005) was modified slightly to account for differences in formation thickness and the possibility of occurrence of a CO₂ front during the flow. With this conceptual framework and other assumptions based on the Nordbotten solution (Nordbotten et al., 2005), the following equation, which governs the flow of composite fluid over the entire AZMI thickness, was derived:

$$-kB\nabla \cdot (\lambda \nabla \bar{p}) = Q_{\alpha}^j \delta(X - X_{well}) \quad (11)$$

where, B is the thickness of the AZMI, λ is the total mobility [M⁻¹LT], $\bar{p}$ is the vertically averaged pressure governing the flow of the composite fluid, δ is the Dirac delta function, and $(X - X_{well})$ is the distance to the location of k-means centroid or the “pseudo injection points” from corresponding point X .

The individual phase mobility is defined as the relative permeability of the phase to that of fluid viscosity, $\lambda_{\alpha} = k_{r\alpha} / \mu_{\alpha}$.

A general schematic of this flow system is shown in Figure 2. The continuous solution to Equation (11) was derived as follows:

$$P(r, t) - P_0 = -\frac{Q_{\alpha}^j}{2\pi \lambda_{brine} k} \int_{r_{well}}^R \frac{dr}{r[(\lambda - 1)b(r) + B]} \quad (12)$$

$$\int_0^B \phi \pi r^2 db = \int_0^t Q_{\alpha}^j(t) dt = V(t) \quad (13)$$

The thickness b of CO₂ plume was derived as a function of radial distance(r), as follows:

$$\frac{b(r, t)}{B} = \frac{1}{\lambda_{CO_2} - \lambda_{brine}} \left[\sqrt{\frac{\lambda_{CO_2} \lambda_{brine} V(t)}{\phi \pi B r^2}} - \lambda_{brine} \right] \quad (14)$$

and,

$$\lambda = \frac{b}{B}\lambda_{CO_2} + \frac{(B-b)}{B}\lambda_{brine} \quad (15)$$

To reduce the computational time of the model, we break the non-linear, second order ordinary differential form of the solution into a step-wise form. Thus, the solution to Equation (11) can be represented, as shown below, to predict CO₂ pressure response:

$$\left| P_{CO_2}(r, t) - P_0 \right|^j = \begin{cases} -\frac{Q_{CO_2}^j}{2\pi KB} \left\{ \frac{1}{\lambda_{CO_2}} \ln \left(\frac{r}{a_2} \right) + \left[\frac{B}{b\lambda_{CO_2} + (B-b)\lambda_{brine}} \right] \ln \left(\frac{a_2}{a_1} \right) + \frac{1}{\lambda_{brine}} \ln \left(\frac{a_1}{R} \right) \right\}, & r_{well} < r < a_2, \\ -\frac{Q_{CO_2}^j}{2\pi KB} \left\{ \left[\frac{B}{b\lambda_{CO_2} + (B-b)\lambda_{brine}} \right] \ln \left(\frac{r}{a_1} \right) + \frac{1}{\lambda_{brine}} \ln \left(\frac{a_1}{R} \right) \right\}, & a_2 < r < a_1, \\ -\frac{Q_{CO_2}^j}{2\pi KB} \left\{ \frac{1}{\lambda_{brine}} \ln \left(\frac{r}{R} \right) \right\}, & a_1 < r < R. \end{cases} \quad (16.3)$$

where, R is the outer boundary of the domain and,

$$a_1 = \sqrt{\frac{\lambda_{CO_2} V(t)}{\phi\pi(b\lambda_{CO_2} + (B-b)\lambda_{brine})}} \quad a_2 = \sqrt{\frac{\lambda_{brine} V(t)}{\phi\pi(b\lambda_{CO_2} + (B-b)\lambda_{brine})}} \quad (17)$$

Equations (16.1 – 16.3) calculate the changes in pressure from fluid migration into the AZMI for the j^{th} cluster. We then use superposition of the pressure change response vectors resulting from the flux aggregation of each of the clusters to compute the cumulative pressure change in the AZMI (ΔP_{AZMI}).

$$\Delta P_{CO_2}^j = \left| P_{CO_2}(r, t) - P_0 \right|^j$$

$$\Delta P_{AZMI} = \sum_{j=1}^k \Delta P_{CO_2}^j \quad (19)$$

2.6. Fluid Properties

Fluid properties such as density and viscosity may have an important role in the quantification of fluid flow in a porous media. These properties of CO₂ are functions of temperature and pressure of the formation, which in turn are functions of its depth. The density and viscosity of brine are functions of salinity as well. Therefore, to compute the fluid properties, the temperature and pressure for the formation were assumed to have a gradient of 0.025°C/m and 0.01 MPa/m, respectively (Raza, 2009; Szulczewski and Juanes, 2009). Depending on the depth of the AZMI formation; the AZMI ROM calculates the fluid properties based on look-up tables. The look-up tables were generated using recent equation-of-state publications on pure water, saline solutions, and CO₂ over a range of 0.10 to 60 MPa, 0 to 180°C, and 0 to 80,000 ppm salinity (Lemmon et al., 2010; Wagner and Pruss, 2002; Huber et al., 2009; Span and Wagner, 1996; Fenghour et al., 1998). Since the impact of CO₂ dissolution in brine has been ignored in this work, its impact on the density of brine does not play a role (Meng and Jiang, 2014).

3. BASE CASE ANALYSIS

3.1. AZMI Model Base Case Setup

A hypothetical AZMI system was defined and is used as the subject of base case analysis. This system consists of AZMI layer overlying a 10-m thick primary seal and 100 m thick storage reservoir. The reservoir is located at a depth of 1000 m. The areal extent of the subsurface storage system is defined as 10 kms × 10 kms. The reservoir and seal features used in this study are shown in Table 1. CO₂ is injected into the storage aquifer at a rate of 1 MT per year for a period of 30 years. CO₂ and brine flux from the seal are simulated for a period of 30 years of injection and 170 years of post-injection using TOUGH2. It is assumed that the AZMI layer has a porosity of 0.1 and a permeability of 10.5 mD. The residual CO₂ and brine saturations were set at 0.01 and 0.02 respectively and the bubbling pressure was set to equal 0.01 MPa. The reference CO₂ and brine viscosities, and CO₂

and brine density corresponding to the AZMI were calculated from the lookup tables as described in Section 2.6. The study addresses two different AZMI scenarios of varying thickness. The Scenario I is based on a 3-m thick AZMI and the Scenario II is based on a 90 m thick AZMI. Figure 3 describes the geologic profile of these benchmark storage scenarios.

3.2. TOUGH2 Model Description

The AZMI ROM takes its input in the form of fluid flux from the underlying seal. Any full-scale reservoir simulator such as TOUGH2 (Pruess et al., 2012) or ROM such as NSealR (Lindner, 2015) can be used to generate these fluid flux inputs for the AZMI ROM. In this study, we use a detailed TOUGH2 simulation to compute the flux output from the seal and used the outputs as an input to the AZMI ROM.

TOUGH2 is a multi-phase flow transport code that has been widely applied to simulate subsurface migration of CO₂ and brine under geologic carbon storage conditions (Oldenburg et al., 2001; Pruess, 2008; Zhou et al., 2010; Rohmer and Seyed, 2010; Zhang et al., 2016). In this study, a 3-D TOUGH2 model was developed to simulate the injection of CO₂ into a deep saline reservoir, as well as CO₂ and brine leakage through the seal based on its intrinsic permeability. The model was constructed with five vertically stacked horizontal intervals as shown in Figure 4. Moving from bottom to top, these intervals were comprised of a lower boundary, the CO₂ storage reservoir, the seal, the AZMI and an upper boundary. The dimensions of the modeling domain were either 10,000 m × 10,000 m × 133 m (Scenario I) or 10,000 m × 10,000 m × 220 m (Scenario II). The upper and lower boundary intervals had very low permeabilities (10^{-19} m² for horizontal permeability and 10^{-20} m² for vertical permeability), and a thickness of 10m each. Adding together the upper and lower boundaries (20m), the storage formation (100m), the seal (10m), and the AZMI thicknesses of 3m and 90m yields thicknesses of 133 and 220 m for Scenario I and II, respectively. The CO₂ was injected into the CO₂ storage reservoir, which was 100m thick. The interval above the CO₂ storage reservoir was the seal interval, which is 10m thick. The portion of the seal blocks representing a

non-fractured seal had a horizontal permeability of 10^{-19} m^2 and a vertical permeability of 10^{-20} m^2 ; portion of the seal blocks representing a fractured seal had an identical horizontal permeability but a vertical permeability of 10^{-17} m^2 . The interval above the seal was designated as the AZMI, which had a porosity of 0.1 and a horizontal permeability of 10.5 mD. In the central region surrounding the CO_2 injection well, small grid blocks were assigned to capture the complex two-phase transport behavior that would take place close to the injection well. Grid blocks with larger sizes were assigned in other regions outside the central region. The model had 23,328 active grid blocks in total for Scenario I and 37,908 active grid blocks in total for Scenario II.

3.3. Results from AZMI ROM

For demonstration purpose, a credible, but arbitrarily selected, heterogeneous seal permeability was used for the model input of the base case as represented graphically in Figure 5. The same seal permeability has been used for the TOUGH2 simulations. The higher permeable zones in the test case have permeabilities that are three orders of magnitude greater than those of the low permeable zones of the seal. The higher permeability zones in the seal are taken to be representative of leaky zones. It is expected that fluid will migrate preferentially through these high permeable zones, as would also be expected in fractured zones of a caprock. The fluids migrating out of the seal through the high permeable zones then move through the overlying porous and permeable formation (the AZMI), driven by pressure gradients and buoyancy, resulting in an increase in pressure in the region.

Figures 6 and 7 present the changes in pressure responses in the AZMI over time for Scenarios I and II, respectively, as generated using flux from the seal (TOUGH2 results) for the simulation periods previously discussed. For both scenarios, the highest increase in pressure is observed at the centroids of the high permeable zones at the end of injection (i.e., 30 years), with the maximum increase in pressure being about 0.49 MPa and 0.20 MPa for Scenario I and II, respectively. The change in pressure gradually fades away from the centroids of the high permeable zones to the simulation domain boundaries for both

of the scenarios. After CO₂ injection stops, the rate of increase in pressure gradually decreases and normalizes over time by the end of the simulation (i.e., following a post-injection period of 170 years). Figures 6 and 7 also show that the change in pressure decreases as the thickness of the AZMI increases. The pressure change in the thick AZMI scenario is smaller because the total pore volume into which the additional fluid is moving is significantly greater, so there is more capacity for attenuation of that fluid within the system.

The AZMI ROM also calculates the CO₂ saturation distribution in the AZMI over time. However, the saturation calculation is limited by the fact that the input flux to the AZMI ROM is a 1D flux. As mentioned earlier, the AZMI ROM has been developed to be consistent with the IAM development effort of NRAP, which produces vertical 1D flux from the seal ROM, NSealR (Lindner, 2015). This restricts the ability of the AZMI ROM to predict the lateral spread of CO₂ over time. Future work will include the development of a 1D to 2D flux conversion approach that will permit the more accurate prediction of CO₂ saturation in the AZMI.

For demonstration purpose, in this particular study, we used the 3D flux characterization from TOUGH2 to predict the saturation. In the main AZMI ROM code, we only use the vertical flux (1D) from the seal layer to predict changes in pressure at the top of the AZMI. The purpose of using 3D flux results is that the 1D flux is not able to capture the radial extent of migration of the plume, which is an important requirement to define the saturation profile. From the perspective of informing AZMI saturation, the 1D flux input is, therefore, noted as a significant shortcoming.

Figures 8 and 9 shows CO₂ saturation distribution at the top of the AZMI layer over time for Scenarios I and II, respectively. In Scenario I, the CO₂ plume in the storage interval tends to migrate out beyond the high permeable zones near the injection well. Since the mobility increases over time due to increase in relative permeability of CO₂, the plume tends to disperse more with time and continues to increase even after the injection stops. In Scenario II, the CO₂ plume in the AZMI is more localized compared to the pressure

change and the increase in CO₂ saturation was only seen in the regions very close to the high permeable zones near the injection well. The maximum extent of CO₂ plumes in the AZMI around the high permeable zones near the injection well is shown in the Figures 8 and 9. Since the AZMI thickness is much less in Scenario I compared to that of Scenario II, the mobility of CO₂ near the high permeable zones is much higher in Scenario I and the dispersion rate is quite high. As can be seen from these figures, the maximum extent of the CO₂ plume in Scenario I is 6,350 m compared to that of 3,250 m in case of Scenario II. Considering CO₂ dissolution in the model may reduce CO₂ saturation aerial extent, resulting in slow dispersion of the CO₂ plume.

3.4. Model Validation using TOUGH2

To verify the computational ability of the AZMI ROM, we make a comparison of the AZMI ROM pressure change predictions with those of a comparable TOUGH2 model. Essentially, this verification effort involves using TOUGH2 flux results from the seal as an input to the AZMI ROM, and then comparing the results of the AZMI ROM with that of TOUGH2 outputs for similar intervals of the storage system for both of the base case scenarios. Figures 10 (a) and 10 (b) show comparisons of the pressure responses of the AZMI ROM and TOUGH2 simulator at particular locations in the AZMI for Scenarios I and II, respectively. Locations directly above two of the high permeable seal zones (Grid coordinates (38,63), located 1.769 km northwest of the injection well and (50,19), located 3.1 km south of the injection well), and the location directly above the injection well (grid coordinate (50,50)) were selected to illustrate the important trends. The spatial difference in the two model predictions is also compared at the end of injection (i.e., 30 years) and at the end of simulation (i.e., 200 years) in Figure 11. The absolute pressure deviation is calculated as the absolute difference in the pressure prediction of AZMI ROM to that of the TOUGH2 simulator. Table 2 summarizes the simple statistical analysis carried out for the model comparison using mean absolute percentage deviation.

$$\text{Mean Absolute Percentage Deviation} = \frac{|\Delta P_{AZMI} - \Delta P_{TOUGH2}|}{\Delta P_{TOUGH2}} \times 100\% \quad (20)$$

where, ΔP_{AZMI} is the change in pressure predicted by AZMI ROM and, ΔP_{TOUGH2} is the change in pressure predicted by TOUGH2.

This analysis shows that the results tend to vary, to some small extent, through the period of injection with TOUGH2 predicting higher pressure compared to that of the AZMI ROM. Once injection stops, the AZMI model seems to provide a better match with that of TOUGH2. During the first 10 years of operation, the pressure is higher in TOUGH2 predictions since the TOUGH2 model captures the 3D flow of the CO₂ in the AZMI, resulting in a resistance to the CO₂ flow from all three directions. As such, in the TOUGH2 model, more cumulative pressure is required by the CO₂ to overcome the resistance to replace the brine in the AZMI, as compared to the AZMI ROM where the CO₂ flow is considered only in one dimension. With the increase in injection time, the CO₂ saturation increases, and so does the relative permeability of CO₂. As a result, a lower pressure is required to overcome the resistance to flow with the increase of CO₂ relative permeability. The deviations in predicted pressure response, as can be seen from Figure 11, are greater above the high permeable zones of the seal. Also, it can be seen in Figure 10 (a) that pressure starts decreasing at around 130 years from start of injection. This is the time when CO₂ in the AZMI reaches the system boundary. This behavior is only observed in Scenario I, i.e., the 3 m thick AZMI case. There is no pressure decrease observed in Scenario II because CO₂ plume never reaches the system boundary at the top of 90 m thick AZMI.

Since there have been several model reduction techniques used in the current model development, the minor differences in the models as shown in Table 2, where the mean absolute percent deviation ranges from 0.3 to 1.2%, are expected. These results confirm that the AZMI ROM, which is computationally more efficient than TOUGH2, still provides acceptable accuracy relative to that of the full complexity model. Taking into consideration the fact that discrepancy in the prediction of physical processes can be dominated by uncertainty of subsurface properties (Oladyshkin et al., 2011), however, suggests that these minor differences may not be overly impactful to the predictive utility

of the AZMI ROM. Ultimately, the acceptable degree of deviance from the verifying numerical model will depend on the intended application of this predictive tool, and incorporate some consideration of the trade-off between that deviance and benefit of computation time. For example, a simulation of 30 years in TOUGH2 takes approximately 8 hours of computational time in a stand-alone machine and that of 200 years of simulation takes around 14 – 15 hours of run-time. On the other hand, the AZMI ROM computation times when coupled with seal ROM, NSealR, for these same scenarios are 15 and 34 seconds, respectively, providing an improvement in computation time by a factor of approximately 2000 times.

Generally, it is expected that the computational efficiency and moderate accuracy of the AZMI ROM, as compared to numerical models, will allow consideration of general trends in AZMI response and development of general insights about the value of AZMI monitoring in the context of full system performance, and related uncertainty. It will likely not, however, have application for evaluation of site-specific geologic storage performance, as the model allows only limited functionality to incorporate spatially varying site characteristics. Future work will present the results of performing uncertainty quantification and sensitivity analyses of the system during CO₂ injection and subsequent leakage into the AZMI.

4. CONCLUSION

This work presents a new reduced order model to predict the pressure and saturation response in the Above Zone Monitoring Interval (AZMI). The primary motivation for developing this new model is as a rapid assessment tool to consider the ability to monitor fluid migration into the AZMI in a geologic CO₂ storage setting. This tool can be applied to describe subsurface response to large-scale CO₂ injection, and explore implications of that response for diagnostic purposes of seal integrity, plume disposition and related uncertainties. A flux aggregation approach using a statistical data-clustering algorithm was applied to quantify fluid fluxes of CO₂ and brine into the AZMI. This influx through

the primary seal is distributed throughout the AZMI using a multi-phase fluid flow model based on a simplified version of an existing analytical solution developed by Nordbotten et al. (2005) for CO₂ storage. A benchmark study to describe a credible CO₂ storage scenario was performed using baseline AZMI parameters, and CO₂ and brine flux inputs from the seal TOUGH2 numerical model. The benchmark storage case was also set up in TOUGH2 and fluid migration through the seal predicted. The base case study is used to investigate two scenarios reflecting different AZMI thickness. For both scenarios, comparisons were made between results from the new AZMI ROM and TOUGH2. The AZMI ROM pressure predictions differ from those of TOUGH2 by a maximum of 1.2 % for identical simulation settings. The AZMI ROM tends to under predict in certain cases due to the extensive complexity reduction methodologies that were incorporated into the formulation of the AZMI model. One of the main features of the AZMI ROM is that it is computationally very inexpensive compared to full-scale numerical simulators. In this work, we use fluid fluxes from TOUGH2 as an input to the model. In the future, the model can be coupled with reservoir and seal prediction ROMs in an integrated assessment framework, to complement assessment of whole system performance.

The model for seal permeability applied herein includes simplifying assumptions that could present limitations to its application to more realistic geologic scenarios. Still, the tool provides a practical approach for rapid prediction of general trends in AZMI performance as a function of select uncertain system parameters. It can be used to explore ranges of time-dependent response in AZMI as a function of AZMI characteristics and seal integrity disposition. In addition, one limitation of this model is it does not consider the solubility of CO₂ in brine which can lead to inaccurate model predictions. We also do not consider geomechanical effects. Geomechanics can play an important role in pressure predictions above the seal with some of the well-known effects being stresses and strains on overlying formations due to fluid migration; pressure perturbations due to injection of CO₂; and induced faults and fractures in the system leading to local micro-seismic events (Rutqvist, 2012; Varre et al., 2015). On one hand, pressure build-up in the AZMI can be substantially reduced in case of structural deformation; on the other hand, formation of faults and fractures can lead to more CO₂

and brine migration, which will lead to significant pressure increases above the seal. For these reasons, development of geomechanical reduced order models for future incorporation into the current AZMI ROM is warranted. The AZMI model presented in this study is able to capture the general trends of numerical reservoir modeling. In presence of sitedata, other response surface based ROMs developed using site-specific numerical realizations can be used to model storage scenarios and those model results then can be used by the AZMI ROM to predict geologic behavior more accurately. Through integration with other system component models and application of probabilistic sensitivity and uncertainty quantification approaches, this tool can improve understanding of likely AZMI response in the context of the whole-system, with potential utility to explore value of AZMI monitoring for early leakage detection.

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Figure 1: Integrated Assessment Model (IAM) structure showing position of AZMI ROM in the systems level hierarchy. The model structure acts as a basis to the IAM modeling algorithm where the user defines the storage scenarios, geologic conditions and simulation properties. Each ROM (in red box) passes input to the overlying receptors. The green arrows represent system levels that can be used for monitoring framework design.

Figure 2: Schematic diagram showing: (a) aggregated CO₂ flux at j^{th} cluster (in red) containing “ m ” number of grid blocks (in grey); (b) a typical profile of CO₂ region denoted by $b(r,t)$ in AZMI; and (c) plan view of radial boundaries for step-wise form of pressure as described in Equations (16.1) – (16.3), assuming well location at the center marked in red, a_1 and a_2 are radial coefficients described in Equation (17).

Figure 3: $X = 10$ km Geological profile of the base case CO₂ storage site representing two different AZMI thickness scenarios (*not to scale*).

Figure 4: Configuration of the 3-D TOUGH2 Model. The X-Y view shows small grid blocks in the central region surrounding the CO₂ injection well. The thickness of the CO₂ storage formation is 100 m. The thickness of the AZMI (H) is 3 m for Scenario I, and H is 90 m for Scenario II.

Figure 5: Map view of seal permeability used for the benchmark CO_2 storage site showing coordinates of injection well location of coordinate (50,50) and centroids of two high permeable zones (38,63) located approximately 1.769 km northwest of the injection well and (50,19) located 3.1 km south of the injection well.

Figure 6: Change in pressure response (in MPa) at the top of AZMI for Scenario I (thickness of 3 m) through 200 years of total performance (including 30 years of injection).

Figure 7: Change in pressure response (in MPa) at the top of AZMI for Scenario II (thickness of 90 m) through 200 years of total performance (including 30 years of injection).

Figure 8: Saturation response at the top of AZMI (thickness of 3 m) through 200 years of total performance (including 30 years of injection). The spatial extent of gas plume at the end of simulation is also shown.

Figure 9: Saturation response at the top of AZMI (thickness of 90 m) over time through 200 years of total performance (including 30 years of injection). The spatial extent of gas plume at the end of simulation is also shown.

Figure 10: Pressure prediction comparison between AZMI ROM and TOUGH2 at three locations: coordinate (38, 63), located approximately 1.769 km northwest of the injection well, coordinate (50, 19), located 3.1 km south of the injection well and, coordinate (50, 50) at the injection well, at the top of AZMI for (a) Scenario I (thickness of 3 m) and (b) Scenario II (thickness of 90 m) over time. The dashed line represents the time when CO₂ injection ends (t=30 years).

(a)

(b)

Figure 11: Absolute deviation in pressure prediction between AZMI ROM and TOUGH2 simulations at the end of 30 and 200 years for AZMI thickness (a) = 3 m (b) = 90 m.