Numerical modeling study of the CO₂ trapping characteristics of thin-skinned fold and thrust belts: a case study of the Catawba Syncline, Virginia, U.S.A.
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Summary
Carbon capture and storage (CCS) is a strategy for reducing global greenhouse gas emissions from fossil fuel burning energy generation and industrial processes, like cement and steel production. In the U.S., the Appalachian Basin contains abundant hydrocarbon resources and is the location of numerous industrial facilities, making the region a promising location for CCS development. To improve the understanding of CO₂ trapping mechanisms in the thin-skinned fold-and-thrust belt setting of the Appalachian Basin, this study develops a suite of CCS numerical models for the Catawba Syncline, VA, U.S.A.

Introduction
Carbon capture and storage (CCS) is the process of capturing CO₂ that would normally be emitted in large quantities from hydrocarbon and/or industrial related facilities and storing the captured CO₂ underground in a variety of geologic reservoirs, including depleted hydrocarbon fields, saline reservoirs, and mafic igneous rocks. CCS is rapidly being implemented globally as a means of mitigating carbon emissions, spurred by government incentives and maturing carbon markets.

In the United States, the Appalachian Basin has historically been the most productive basin for coal extraction and holds significant oil and gas reserves. The basin has produced a cumulative 34.5 billion short tons of coal and holds another 66 billion short tons in reserve (Tewalt and Ruppert, 2014). Additionally, the Appalachian Basin holds 4.76 billion barrels of oil and 124.9 trillion cubic feet of gas in ultimate recoverable oil and gas reserves (Ryder et al., 2014). This extensive hydrocarbon extraction involves numerous facilities with large CO₂ emissions, which could benefit from CCS development.

Therefore, the challenge for CCS development in the Appalachian Basin is not in locating CO₂ sources, but in finding suitable CO₂ storage reservoirs for the captured carbon. Deformation associated with the orogenesis of the Appalachian Mountains, introduces several challenges and opportunities for the implementations of CCS in the region. Specifically, the thin-skinned fold and thrust belt style deformation of the Appalachian Valley and Ridge province, creates complex structural traps that could be utilized for geologic carbon sequestration. However, the complex geology and limited seismic exploration in this region, presents difficulties for finding suitable structural traps. This paper explores one such structural trap for CCS, the Catawba Syncline, using numerical modeling methods. Our results indicate that fold and thrust belt geologic architecture can effectively trap commercial-scale volumes of injected CO₂ for long-term geologic sequestration.

Method
The Catawba Syncline was selected as the study area of this project, based on its proximity to local industrial emitters, the presence of a potential reservoir-seal system, and its thin-skinned fold and thrust belt geology. The Catawba Syncline is a doubly plunging synclinal structure in southwest Virginia that extends from Blacksburg, VA to the North of Roanoke, VA (Figure 1). It is bounded by the Pulaski thrust system, which displaces the Cambrian Rome formation over younger Mississippian and Devonian units (Bartholomew, 1987; Bauerlein, 1966; Broughton, 1971). It is unknown whether there is additional blind thrust faulting, below the Pulaski-thrust sheet in the Catawba Syncline.

Figure 1: Approximate location of study site in southwestern Virginia, U.S.A., shown in upper left. The surface expression of the Catawba syncline is indicated by the red box in the satellite image (modified from Google Earth).

Due to the lack of deep wells or seismic reflection surveys in the study area, three kinematically feasible cross-sections were developed for the subsurface based on surface outcrop mapping (Figure 2). Scenario 1 represents geologic conditions with no additional deformation below the Pulaski thrust sheet. Scenarios 2 and 3 each feature blind thrusting
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and associated folding beneath the Pulaski Thrust Sheet, with detachment occurring in either the Martinsburg Formation (scenario 2) or in the Rome Formation (scenario 3). Scenario 1 represents the worst-case scenario in terms of CO₂ trapping as there are no geologic structures to impede the flow of CO₂ up the arm of the syncline. Scenarios 2 and 3 likely represent more favorable geologies as the fold and thrust structures create barriers to CO₂ flow. In all three scenarios the Millboro shale (dark blue, Figure 2) is expected to behave as a stratigraphic trap, limiting buoyancy-driven CO₂ flow.

The Oriskany Sandstone and Millboro Shale formations were identified as a potential reservoir-seal system on the basis of their ability to hold hydrocarbons in fields near our study site. The Bergton gas field in Rockingham County, VA, is one such site. At Bergton, a large anticlinorium with minor folds and thrust fault structures trap natural gas in the Oriskany formation (Young and Harnsberger 1955). This site is located in the thin-skinned fold and thrust belt section of the Appalachian basin (Valley and Ridge Province), and has similar geologic features to the Catawba Syncline, e.g., a large fold structure compounded by thrust faults and associated minor folds. Therefore, it may be a useful analog for the Catawba Syncline, in the absence of local drilling and core analysis. Furthermore, analysis on Oriskany core from the Bergton field indicate porosities of 10.9 – 12.2 % and average permeabilities of 14.7 md (1.45E-14 m²), which suggest the rock has properties suitable for geologic CO₂ storage (Simmons, 1983). The Midwest Regional Carbon Sequestration Partnership (MRCSP) also conducted a carbon storage resource assessment on the Oriskany and found that the unit holds approximately 19.429 gigatons of CO₂ storage potential, but their assessment did not include Virginia (Wickstrom et al., 2005). Nevertheless, the assessment further supports the Oriskany as a potential carbon storage reservoir. The Millboro formation is a tight black shale that is upwards of 300 ft thick in this part of the Appalachian Basin and has low permeabilities suitable for preventing fluid flow (Enomoto et al., 2014). Based on these assessments, the Oriskany and Millboro formations were used as the target reservoir and primary seal for this modeling study.

These rock properties and the three geologic scenarios were each digitized into model meshes with 420,000 cubic grid cells with dimensions of 110 m. The model is approximately 19,320 m long in the X axis (northwest-southeast direction), 5,650 m long in the Y axis (northeast-southwest direction), and has a maximum depth of 4,300 m below surface (3,465 below mean sea level). The completion interval for CO₂ injection is located at 2020-2050 m depth below surface, which is within the modeled Oriskany formation. Each model scenario simulates 100 years of CO₂ injection at a constant rate of 862,000 metric tons CO₂/year, which are the approximate emissions of an industrial emitters in the region. The models were then relaxed, i.e., the simulation continued without CO₂ injection, for 1,000 years to study post-injection behavior. The models were constructed using the simulation software, PetraSim (RockWare, 2022) and

![Figure 2](image_url)

Figure 2: Three kinematically feasible cross-sections for the Catawba syncline and their associated model meshes. The dark red unit represents Cambrian carbonate basement rocks, including the Rome formation. The orange unit represents Ordovician shale and limestone units, including the Martinsburg formation. The light blue unit represents the Lower Devonian Oriskany sandstone, which is the target reservoir of this study. The dark blue unit represents the Devonian Needmore and Millboro shales. The purple unit represents the Upper Devonian sandstones and shale units including the Foreknob and Brallier formations. The green unit represents Mississippian age formations.
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Simulations were computed using the TOUGH3 code with the ECO2N v2.0 module for non-isothermal flow of water, CO₂, and NaCl. The TOUGH3 code utilizes an integral finite volume method in space and a first-order finite difference method in time to solve the mass and energy conservation equations (Jung et al., 2017; Pan et al., 2017; Pruess and Spycher 2007).

Simulation results suggest that the Catawba syncline is a suitable location for CCS in all three geologic scenarios. Under these model conditions, injected CO₂ migrates up-dip due to buoyancy, but did not leave the super-critical phase and/or leak to the surface. Therefore, with these model parameters there is little risk of CO₂ leakage through surface outcrops of the Oriskany sandstone after 1,000 years. The nature of CO₂ plume propagation in the simulations varied significantly based on its geologic scenario (Figure 3, Figure 4).

In scenario 1, CO₂ migrated away from the well, primarily in the up-dip direction. After 100 years of injection, the CO₂ plume reached a maximum length in the X direction of 3,705 m (Figure 3) and a length of 2,095 m in the Y direction. Because there are no structures to trap the CO₂, the plume continued to migrate up-dip during the post-injection period, reaching an X direction length of 7,960 m (Figure 4) and a Y direction length of 2,176 m. The CO₂ plume stabilized and stopped migrating after 784 years, post-injection, when the buoyancy-driven CO₂ flow no longer had sufficient pressure to overcome the capillary force of the in-situ pore fluid. The CO₂ plume reached an up-dip depth of 1,230 m below surface, which is still at sufficient pressure and temperature conditions to keep the CO₂ in the supercritical phase. While this scenario is technically successful in storing the injected CO₂, we note that the large lateral diameter of the CO₂ plume would result in a large area of review for a commercial storage project, presenting difficulties in terms of monitoring and verification.

In scenarios 2 and 3, the structural geometries trap a large percentage of the injected CO₂, limiting the up-dip migration of the plume. After 100 years of injection, the CO₂ plume in scenario 2 has a length of 3,160 m in the X direction (Figure 3) and 2,295 in the Y direction. The CO₂ plume in scenario 3 has a length of 3,465 m in the X direction (Figure 3) and 2,435 m in the Y direction. After 1,000 years of post-injection simulation, the CO₂ plume in scenario 3 has a length of 3,790 m in the X direction (Figure 4) and 4,515 m in the Y direction. The post-injection plume for scenario 4 is 4,240 m long in the X direction (Figure 4) and 5,420 m long in the Y direction. In these two scenarios, the fold and thrust structures limited the up-dip flow of CO₂, resulting in further migration in the Y direction. Our geologic models assume constant geology along the Y axis (NE-SW direction); however, it is possible that minor faults or folds exist in the Syncline that may compartmentalize the area into discrete sections, significantly altering CO₂ flow patterns.

**Conclusions**

These results suggest that fold and thrust-belt structures, such as the blind thrusting and associated folding in scenarios 2 and 3, create suitable traps for limiting CO₂ plume migration; however, it is clear that CO₂ trapping in these environments will require careful volumetric analysis for durable CO₂ storage.

For the United States to reach net-zero CO₂ emissions, it is necessary to implement CCS in the Appalachian Basin. However, the complex structure and lack of subsurface exploration, present notable challenges for CCS development. Our results support the feasibility of CCS in one area of the basin, the Catawba Syncline, while also highlighting the potential for CO₂ trapping in fold and thrust belt style structural architecture. These structures may effectively trap CO₂, reducing plume propagation and potentially benefitting projects by reducing leakage risk and decreasing the area of review.

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Figure 3: Simulation results after 100 years of CO\textsubscript{2} injection. In all scenarios injected CO\textsubscript{2} remains in the target Oriskany formation and extends radially from the injection well. Scenario 1 features farther up-dip plume migration than scenarios 2 and 3, due to the lack of the structural straps in scenario 1 geology.

Figure 4: Simulation results after 1000 years of post-injection relaxation. Note that the fold and thrust structures in scenarios 2 and 3 significantly impede the up-dip migration of the CO\textsubscript{2} plume in the post-injection phase.