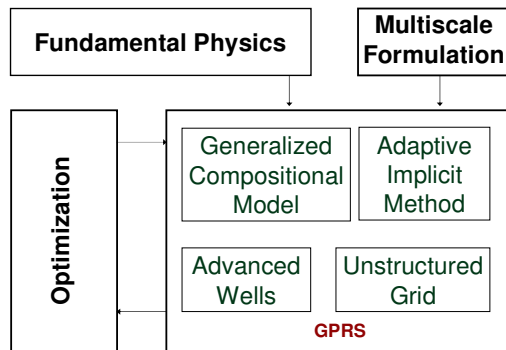


Background

Introduction

Accurate and reliable modeling capabilities for simulating the long-term sequestration of CO₂ will be required. Engineering models will eventually be used in all phases of the sequestration operation; i.e., for site selection, management and optimization during CO₂ injection, and long-term monitoring. To address these needs, and to provide a platform for the incorporation of future research results, we are developing a comprehensive CO₂ modeling capability within Stanford's General Purpose Research Simulator (GPRS). Here, we provide a brief overview of the implementation and testing of some recent GPRS extensions required for modeling CO₂ sequestration in subsurface formations.

GPRS (General Purpose Research Simulator) Framework



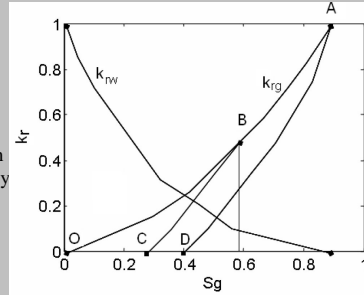
Ongoing GCEP Activities

- Scaling analysis and high-accuracy simulations of miscible and immiscible CO₂ flows.
- High-order AIM (Adaptive Implicit Method) schemes.
- Algebraic finite-volume multiscale formulation.
- Propagation of gravity currents.
- Particle methods for nonlinear multiphase flow.

GPRS Enhancements

Hysteresis

This figure shows typical relative permeability curves of a gas-water system. During CO₂ injection, the relative permeability follows the primary drainage curve O-B-A. As water imbibes, the gas relative permeability will follow a new path B-C. The gas at point C is residually trapped.



Residual trapping of injected CO₂ is generally considered to be safer than structural trapping. This is because, if the aquifer seal is broken, structurally trapped CO₂ may leak, while residually trapped CO₂ is immobile.

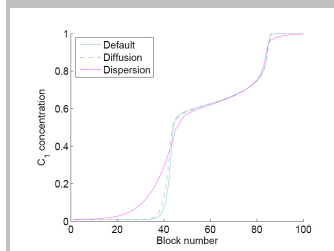
Three different relative permeability hysteresis models were implemented into GPRS: Carlson, Land and Jerauld.

Diffusion and Dispersion

Modeling of the molecular diffusion and mechanical dispersion introduces an additional term in the mass balance equation.

$$\frac{\partial N_i}{\partial t} + \sum_k \nabla \cdot (\rho_k \mathbf{u}_k y_{ik}) - \sum_k \nabla \cdot (\rho_k \phi S_k D_{ik} \nabla y_{ik}) - q_i = 0$$

The third term on the left is called the dispersive flux term, which is driven by the gradient of mole fraction.



In this 1D case, methane is injected at the right end to displace a four-component hydrocarbon mixture. The smoothing effect by physical dispersion is clearly shown for this multi-component compositional case.

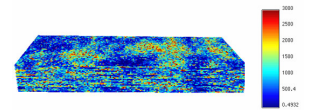
However, current simulation results suggest that dispersion effects do not have a significant impact on the distribution of CO₂ in saline aquifers.

Results

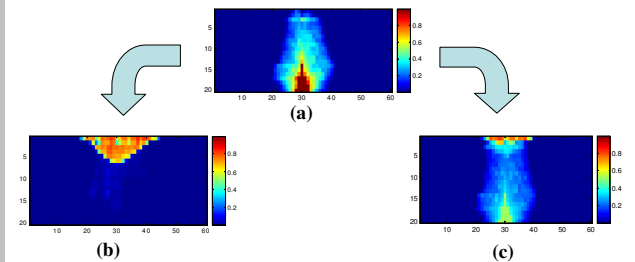
San Juan Saline Aquifer Modeling

We apply GPRS to a model problem derived from an actual saline aquifer, the San Juan saline aquifer in New Mexico, which is under investigation as a potential site of CO₂ sequestration. The model parameters used in the simulations are listed below. The figure shows the permeability field generated for this simulation study.

Parameter	Values
size	262,400 × 98,400 × 1000 ft ³
tops	2000 ft
porosity	0.135
temperature	104 °F
grid	160 × 60 × 20
well location	(100, 30, 20)
avg. permeability	1147 mD



In these simulations, CO₂ was injected at a constant rate of 1.43 BCF/day for 20 years, followed by 80 years of well shut-in, during which the CO₂ migrates due to density contrasts. Figure (a) shows the gas saturation at 20 years. Figure (b) shows the gas saturation 80 years later without hysteresis. Figure (c) is similar to (b), but with hysteresis. Note the huge impact of residual trapping.



Conclusions & Future Work

Stanford's General Purpose Research Simulator (GPRS) was enhanced to include additional effects important for CO₂ sequestration simulations. Now GPRS includes three different relative permeability hysteresis models and the implementation of molecular diffusion and physical dispersion.

Future work:

- Estimate the impact of diffusion and dispersion on practical CO₂ sequestration.
- Test various high-accuracy numerical schemes for modeling CO₂ sequestration.
- Add basic capabilities for dissolution and reactions.
- Demonstrate the use of advanced wells in CO₂ modeling operations.
- Investigate optimization of CO₂ operations using smart wells.