Numerical Solution Schemes for Near-Critical Point Three-Phase Saturation and Relative Permeability

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Abstract

Saline reservoirs selected for the permanent storage of carbon dioxide are generally at depths sufficient to yield pressures and temperatures within the supercritical state for carbon dioxide, yielding a two-phase system; gas and aqueous. Leakage pathways from these deep saline reservoirs to the ground surface experience temperature and pressure conditions that could potentially yield liquid two-phase conditions; nonaqueous liquid and aqueous or three-phase conditions; gas, nonaqueous liquid, and aqueous. The Pacific Northwest National Laboratory is currently developing an extension of its STOMP simulator under the National Risk Assessment Partnership to model the migration of carbon dioxide from deep saline reservoirs to the ground surface via leakage pathways that could include boreholes. The principal objective of this work will be to compare full reservoir simulations against the Open Integrated Assessment Model (OpenIAM). For leakage pathways involving temperature and pressure conditions near the critical point of carbon dioxide, rapid phase appearances, disappearances, and transitions are possible, making numerical solutions in this region difficult. A numerical solution scheme has been developed for the STOMP simulator that smooths discontinuities in capillary pressure, saturation, and relative permeability relationships near the critical point of carbon dioxide via interfacial tension scaling between the nonaqueous-liquid and gas phases. This poster details the developed numerical solution scheme and implementation in the STOMP simulator.

Background

STOMP is a suite of numerical simulators, developed by the Pacific Northwest National Laboratory, for investigating coupled thermal, hydrologic, geochemical and geomechanical processes in geologic media. The suite of simulators comprises a variety of operational modes, each directed at specific application areas. The STOMP-CO2 operational mode was designed for investigating the injection and long-term storage of CO_2 in deep saline reservoirs, considering the four principal trapping mechanisms; dissolution, mineral, hydraulic, and permeability. Whereas this operational mode has been applied against a span of carbon sequestration applications (White et al., 2016; Hou et al., 2012; Bacon et al., 2016, Nguyen et al., 2017), it is strictly a two-phase code, allowing for the modeling of aqueous and nonaqueous systems; where aqueous is assumed to be the wetting phase. Leakage of CO_2 from deep saline reservoirs has the potential of forming three-phase conditions, with aqueous, nonaqueous liquid, and gas phases being simultaneously present. To model these conditions, along with the migration of CO_2 to the ground surface, a new operational mode of STOMP is under development, referred to as STOMP-SEQ. This operational mode extends the capabilities of STOMP-CO2 to three phases, plus air as a component.

At temperature and pressure conditions away from the critical point of CO_2 along the saturation line between the triple point and critical point (see Fig. 1), the thermodynamic and transport properties of liquid and gaseous CO_2 are distinct, making it possible to solve these conditions via classical three-phase saturation and relative permeability functions (White et al., 2004). For temperature and pressure conditions near the critical point of CO_2, however, the physical properties of the nonaqueous liquid and gas become less distinct, and the founding concepts of the classical three-phase modeling approaches become less valid. To address this situation a temperature dependent function for the interfacial tension between liquid and gaseous CO_2 is employed in the solution scheme, allowing for smooth transitions in saturation and relative permeability near the critical point of CO_2. As with other operational modes of STOMP, STOMP-SEQ uses primary variable switching to accommodate phase appearances, disappearances, and transitions. STOMP-SEQ is a nonisothermal, four-component simulator and thus solves five conservation equations for each grid cell, using an implicit finite-volume numerical scheme. For three-phase conditions, the classical pressure approach uses the three phase pressures as the primary unknowns. Phase saturations are then computed via capillary pressure scaling (White et al., 2004):

$$\overline{\overline{s_l}} = f(\beta_{nl}\,[P_n - P_l]);\ \overline{\overline{s_t}} = f\left(\beta_{gn}\,[P_g - P_n]\right) \qquad (1)$$

where, $\overline{\overline{s_l}}$ and $\overline{\overline{s_t}}$ are the apparent aqueous and total liquid saturations, and $\beta_{nl} = \frac{\sigma_{ref}}{\sigma_{nl}}$ and $\beta_{gn} = \frac{\sigma_{ref}}{\sigma_{gn}}$ are the nonaqueous liquid to aqueous and gas to nonaqueous liquid capillary pressure scaling factors, respectively.

Scheme

The classical pressure approach uses capillary pressure scaling to compute the aqueous, nonaqueous liquid, and gas saturations with a single function by scaling the capillary pressures with interfacial tensions. Quinn (1927) reported measurements of the surface tension between gas and liquid CO_2 as a function of temperature along the saturation curve from the triple point (P_t) to the critical point (P_c), as shown in Fig. 2. Unfortunately a straightforward application of the classical pressure scheme would yield an infinite gas-nonaqueous liquid scaling factor. To avoid this singularity, STOMP-SEQ uses a modified pressure approach; where the gas-brine interfacial tension, as reported by Bachu and Bennion (2009), is used to determine the aqueous and total nonaqueous saturation from the gas and aqueous capillary pressure and scaling factor, and the gas saturation fraction is chosen as a primary variable:

$$\beta = \frac{s_g}{s_g + s_n};\ P_n = \frac{P_l\,\sigma_{gn} + P_g\,\sigma_{nl}}{\sigma_{gn} + \sigma_{nl}}$$

where, P_n approaches P_g as the temperature approaches the critical point and the CO_2 surface tension approaches zero. As with the relationships between capillary pressure and phase saturation, the relationships between phase saturations and phase relative permeabilities change with the nonaqueous liquid and gas interfacial tension. As this interfacial tension approaches zero the curvature of the nonaqueous liquid and gas relative permeability curves vanishes and the irreducible saturations drop to zero (Asar and Handy, 1988).

National Risk Assessment Partnership Connection

An important application of STOMP-SEQ will be to create a benchmark case for comparison to NRAP's Integrated Assessment Model (OpenIAM) for scenarios involving leakage from deep saline reservoirs with and without wellbores. OpenIAM is an open-source Integrated Assessment Model (IAM) for phase II of the National Risk Assessment Partnership (NRAP). The goal of this software is to go beyond risk assessment into risk management and containment assurance. The OpenIAM software comprises three distinct components: aquifer, wellbore, and reservoir. The STOMP-SEQ software will provide a benchmark solution that fully integrates these components:

- Aquifer Component - Determine the impact that carbon dioxide (CO_2) and brine leakage from a CO_2 storage reservoir might have on overlying aquifers. An aquifer component predicts the size of "impact plumes" according to water quality metrics such as pH and TDS.
- Wellbore Component - Determines leakage rates to an aquifer component based on pressure and saturation in a reservoir component
- Reservoir Component - Predicts pressure and CO_2 saturation in a storage reservoir based on a specified CO_2 injection rate with time

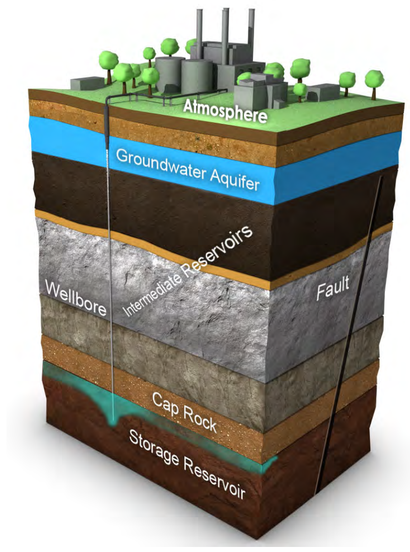

Figure 3. OpenIAM Component Model

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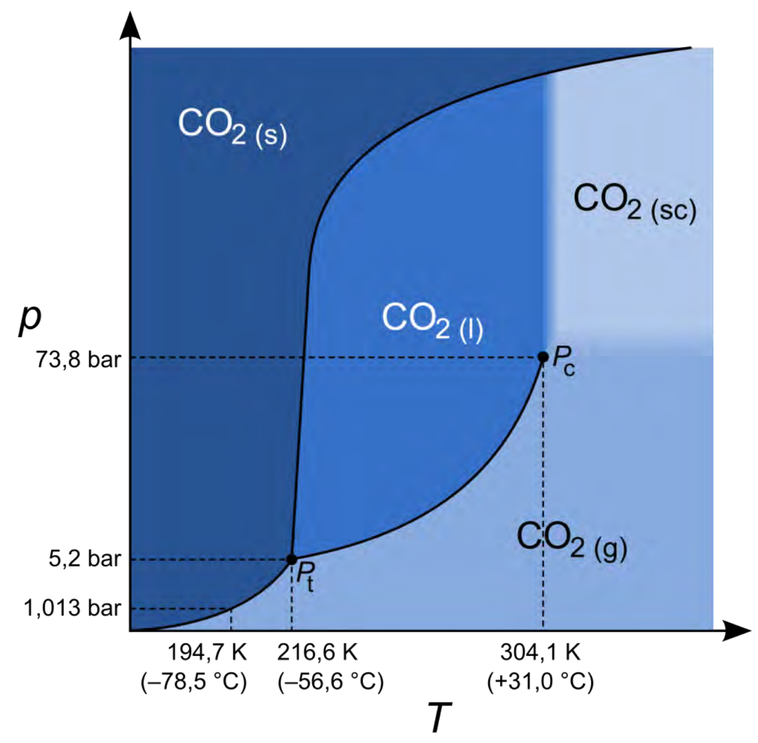

Figure 1. CO_2 Pressure-Temperature Phase Diagram

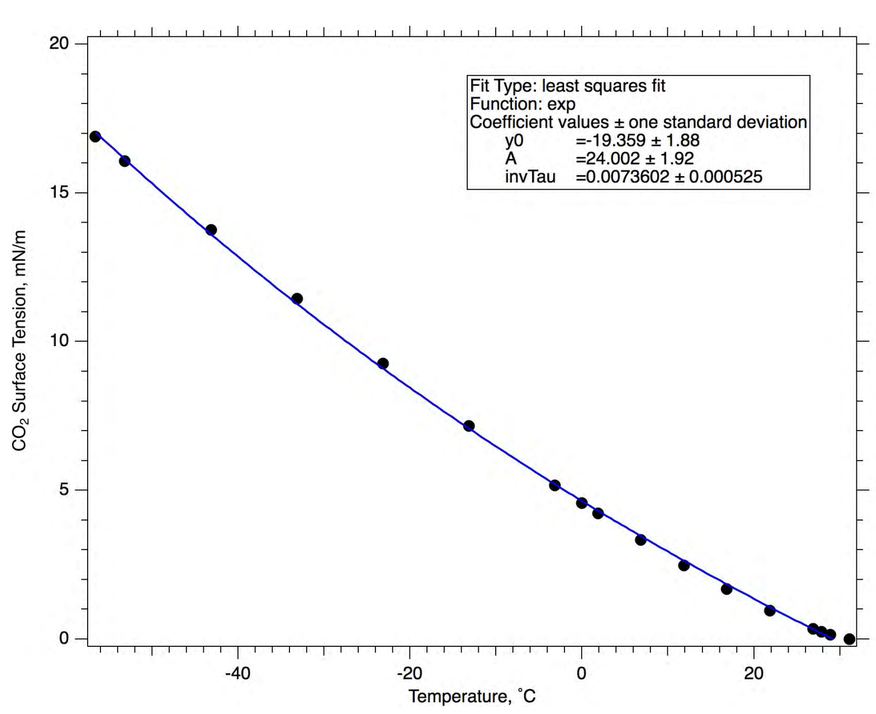

Figure 2. CO_2 Surface Tension between P_t and P_c

ABOUT

Pacific Northwest National Laboratory

The Pacific Northwest National Laboratory, located in southeastern Washington State, is a U.S. Department of Energy Office of Science laboratory that solves complex problems in energy, national security, and the environment, and advances scientific frontiers in the chemical, biological, materials, environmental, and computational sciences. The Laboratory employs nearly 5,000 staff members, has an annual budget in excess of $1 billion, and has been managed by Ohio-based Battelle since 1965.

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