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Modern Phenomenological Methods and Correlations for Estimating Density and Sonic Velocity of Liquid, Gas, and Supercritical CO_2 for Enhanced Assessment of Borehole Acoustic and Seismic Measurements

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Abstract

Petrophysical measurements and their predictions are essential for characterizing the lithology, porosity, and fluid content of CCS reservoirs—a requirement for designing an effective injection and monitoring program. Numerous methods exist for predicting density, acoustic velocity, and other mechanical properties of fluids under various pressure, temperature, and fluid composition conditions. Each method has challenges and limitations, typically relying on equations of state (EOS), empirical correlations, or both. This paper compares approaches for estimating CO_2 density and acoustic velocity at gas/supercritical phase transition zone and deeper storage reservoir depths. The objective is to identify the methods that best predict measurements and lead to accurate petrophysical interpretations for relevant CCS conditions. Four methods are investigated: HSB based on Han et al. (2010) and Batzle-Wang (1992), Peng Robinson (PR) EOS, Perturbed Chain Statistical Associating Fluid Theory (PC-SAFT) EOS, and NIST (REFPROP). Property predictions are compared with lab measurements. Gassmann fluid substitution (1951) is used to propagate errors to derived petrophysical properties including bulk modulus, compressional and shear velocities, V_p/V_s ratio, and horizontal-to-vertical stress ratio as a function of porosity and partial CO_2 saturation.

In the phase transition zone, the REFPROP method results in the least error in density and velocity, as well as in derived petrophysical properties. The HSB method can lead to density (based on Batzle and Wang, 1992) and velocity errors of up to 40% and 25%, respectively, yet usually these errors typically generate less than 1% error in derived petrophysical properties. The HSB errors are more reduced away from the supercritical P-T point. Both PR and PC-SAFT consistently yield derived property errors above 1%. At reservoir storage depths, REFPROP also yields the most accurate results in density and velocity, although PR also performs well. HSB generates some petrophysical property errors above 1%. PCSAFT leads to the

least accurate property estimations. These results show that REFPROP provides the most accurate predictions for CO_2 density and acoustic velocity in transition zone and CCS reservoir storage depths, leading to petrophysical property estimations with errors less than 0.5%. Because HSB is a popular method, it is important to show that significant errors that exist in the HSB density and velocity predictions can result in moderate errors on the order of a 2 to 3% in petrophysical parameter estimation, which can affect 4D seismic/VSP monitoring feasibility assessments.

Introduction

Designing an effective injection and monitoring program relies on accurate petrophysical measurements and predictions. Sonic logging is crucial for estimating mechanical properties that are important for determining where to sample reservoir fluids, pore pressure, and minimum horizontal stress. Sonic logging is also critical for seismic/VSP feasibility assessments, which address the question whether the injection of CO_2 into the reservoir will create a change in seismic reflectivity that would be detectable given the expected injection volume and environmental/survey design noise. If it is detectable, the information further indicates the minimum vertical thickness of the plume, which may practically control the lateral detectability of the plume. Accurate interpretation of sonic logging measurements often requires a fluid substitution calculation to remove the impact of unexpected fluid in the pore space. Such calculations require accurate predictions of the compressional velocity and density of the formation's mineral constituents and pore fluids. The fluid properties are strongly dependent on composition, pressure, and temperature. There are different methods for predicting the density and acoustic velocity of fluids relying on equations of state (EOS), empirical correlations, or both. This paper focuses on pure CO_2 properties.

A popular model for estimating CO_2 is from a software package called *FLAG-2019* published by the University of Houston. FLAG-2019 used the Betzel and Wang (1992) density model and Han et al. (2010) velocity model. Han et al. (2010) made sound wave velocity measurements of CO_2 from 7MPa to 100 MPa. Around the supercritical point (31.1°C and 7.38 MPa), they only made measurements at 7.0MPa and 8.0MPa. It is also well known that it is difficult to control equilibrium around the supercritical state, so elastic properties are exceptionally sensitivity to pressure and temperature. They developed velocity and density models of CO_2 based on experimental data and described the relationships between CO_2 velocity, temperature, and pressure. Using cubic equations of state (EOS) offers advantages in predicting many fluid properties across various pressures and temperatures. Cubic EOS, such as the Peng-Robinson EOS (Peng and Robinson, 1976), enable modeling fluid behavior while honoring fundamental thermodynamic principles. However, these equations often require correlations to improve the accuracy of density calculations. Furthermore, without caloric data, the derived sonic velocities may be inaccurate and traditional cubic EOS, such as PR, also require additional correlations to estimate constant pressure heat capacities under ideal gas conditions. Recently, equations of state such as the Perturbed-Chain Statistical Associating Fluid Theory (PC-SAFT) (Gross and Sadowski 2001) incorporate Helmholtz free energy physics and, thus, model thermal and caloric properties without the need for additional correlations. Alternatively, the NIST developed the Reference Fluid Thermodynamic and Transport Properties Database (REFPROP) for estimating the properties of fluids utilizing models for predicting properties such as density, viscosity, and enthalpy with high precision for a wide range of fluids and mixtures (Huber et al., 2022).

Methods

This study investigates four methods for predicting fluid properties: HSB correlations (implemented in *FLAG* versions prior to 2019), Peng Robinson (PR), PC-SAFT, and REFPROP. The PR and PC-SAFT EOS have been implemented as described by Ahmed (2013) and Gross et al. (2001), respectively. These implementations allow for calculation of compressibility factor, $z(P, T)$, its partial derivatives, and the density and, hence, the speed of sound as follows:

$$v_{sound} = \sqrt{\frac{z(P,T)\left(\frac{c_P(P,T)}{c_v(P,T)}\right)\frac{RT}{M}}{1-\left(\frac{P}{z(P,T)}\right)\left[\frac{\partial z}{\partial P}\right]_T}}, \quad (1)$$

provided one has constant pressure and volume heat capacities, $c_p(P, T)$ and $c_v(P, T)$, respectively. The variables M, R, P, and T correspond to the molar mass, gas constant, pressure, and temperature, respectively. The enthalpy of the fluid, $H(P, T)$, is determined in PC-SAFT, which enables one to directly calculate c_p:

$$c_P = \left[\frac{\partial H}{\partial T}\right]_P. \tag{2}$$

For the PR method, a correlation between the ideal gas constant pressure heat capacity and temperature, $c_p^0(T)$ (superscript *0* refers to ideal gas condition), from Sandler (2017), is used to calculate c_p:

$$c_P = c_P^0(T) - \left(\frac{RT}{\Delta T^2}\right)\int_0^P \frac{z(P,T)T}{P}\,dP. \tag{3}$$

Finally, one can calculate the constant volume heat capacity as follows:

$$c_v = c_P - \left(\frac{R}{P^2}\right)\frac{\left(\left[\frac{\partial zT}{\partial T}\right]_P\right)^2}{\left[\frac{\partial zP}{\partial P}\right]_T}, \tag{4}$$

where the subscripts P and T indicate the partial derivatives are calculated for constants P and T.

Results

The predictions from the four methods are compared against laboratory measurements (Han et al., 2010, Nazeri et al., 2017, Park et al., 2020). For example, Figures 1(a) and 1(b) compare CO_2 density and compressional velocity estimates with measurements at 57°C and 50°C, respectively. One can see density and velocity errors of up to 40% and 20% for some pressures, respectively. To investigate the impact on rock mechanical property assessment of CCS reservoirs, Gassmann fluid substitution is used to assess the propagation of errors to properties including bulk modulus (k), compressional and shear velocities (V_p and V_s), V_p/V_s ratio, and horizontal-to-vertical stress ratio (*HVSR*) both in the dry and partial CO_2 saturation frame. The Eberhart-Phillips et al. (1989) model was assumed with a matrix comprising 80% quartz and 20% clay. Overburden stresses, pore pressures, and temperatures were calculated for 3050 ft depth (transition zone) and 5200 ft depth (supercritical reservoir) assuming Gulf of Mexico subsurface conditions. These values were used to select lab measurements of CO_2 density and velocity as reference answers.

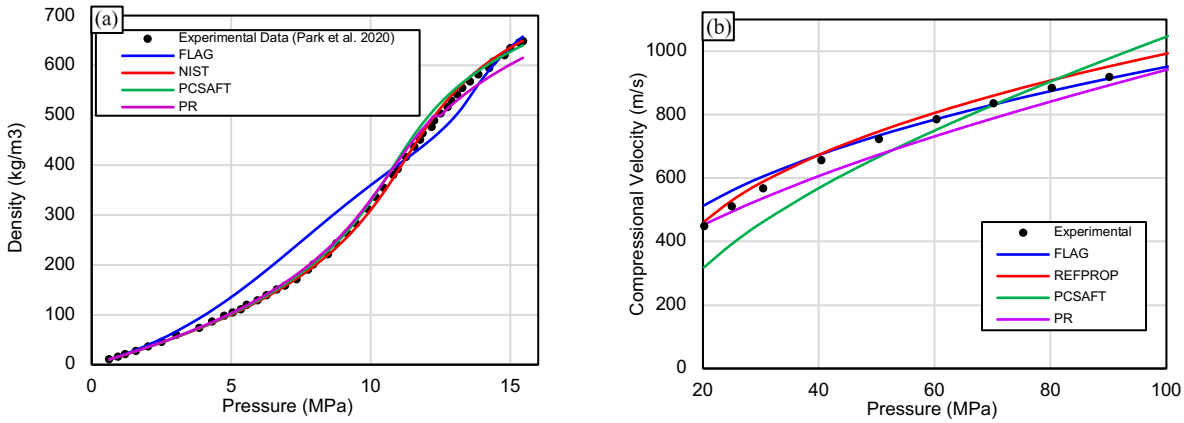

Figure 1. Comparison of density and velocity estimates using FLAG-2019 (HSB), REFPROP, PC-SAFT, and PR equations against experimental measurements at (a) 57°C (Park et al., 2020) and (b) 50°C (Han et al., 2010).

For the partial CO_2 saturation error propagations, a constant porosity of 20% was assumed. As an example, Figures 2(a) and 2(b) show that errors in estimated V_{pSat} and V_{sSat} reach a maximum of 1.3% (PC-SAFT), and 0.5% (HSB), respectively. For the dry frame and *HVSR* error propagations, an initial CO2 saturation of 20% was assumed. As an example, Figures 3(a) and 3(b) show that errors in estimated dry bulk modulus k_{Dry} and *HVSR* reach a maximum of 5% (PC-SAFT) and 6% (PC-SAFT), respectively.

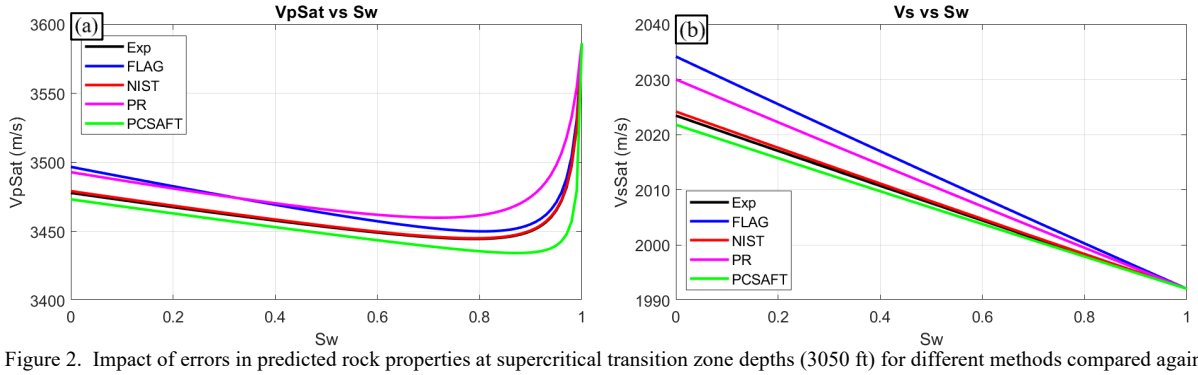

Figure 2. Impact of errors in predicted rock properties at supercritical transition zone depths (3050 ft) for different methods compared against those derived using reference experimental lab fluid property measurements. Errors in *Vp* and *Vs* are assessed by curve offsets from the "Exp" reference curve, which is based on the experimental lab data. Errors reach a maximum of 1.3% and 0.5%, respectively.

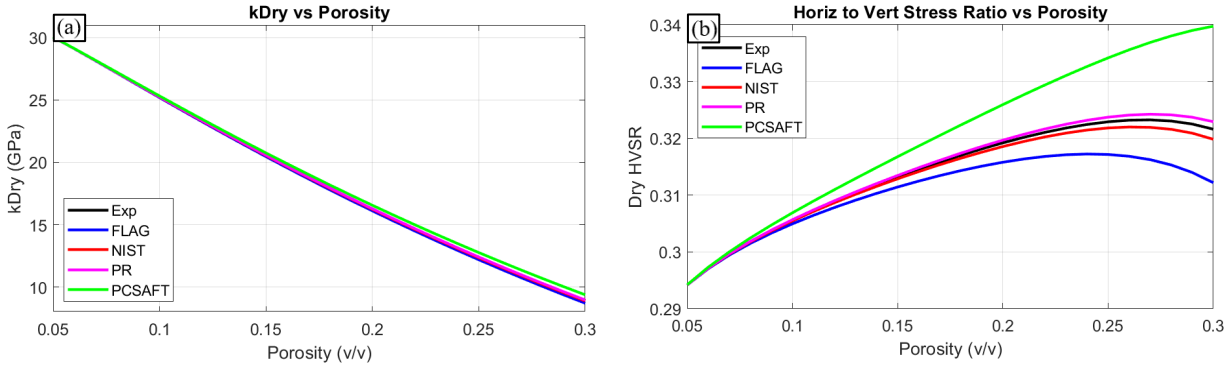

Figure 3. Impact of errors in predicted rock properties at storage reservoir depths (5200 ft) for different methods compared against those derived using reference experimental lab fluid property measurements. Errors in *k* and *HSVR* reach a maximum of 5% and 6%, respectively.

Conclusions

A summary of our numerical modeling investigation is shown in Table 1. The PR and PC-SAFT methods yielded the highest levels of inaccuracy for the bulk moduli and stress ratio calculations. The REFPROP method yielded the most accurate results in all cases. The HSB method yielded accurate results most of the time, but had errors of 2 to 3% in k_{Dry} and *HVSR* at storage reservoir depths. The model developed by Han et al. (2010) has recently been improved. However, since the updates have not yet been published, the results presented in this work refer to the original version.

Type	Property	Transition Zone (3050 ft)				Storage Reservoir (5200 ft)			
		HSB	REFP	PR	PCSAFT	HSB	REFP	PR	PCSAFT
Vary Por	V_{pDry}	-0.3%	0.0%	-1.4%	0.7%	-0.7%	-0.1%	0.0%	1.3%
	V_{sDry}	-0.2%	0.0%	-0.1%	0.0%	0.0%	0.0%	-0.1%	0.0%
	k_{Dry}	-0.6%	-0.1%	**-4.5%**	**2.4%**	**-2.5%**	-0.5%	0.4%	**5.0%**
	HVSR	-0.7%	-0.1%	**-5.4%**	**2.8%**	**-2.9%**	-0.6%	0.4%	**5.6%**
Vary S_w	V_{pSat}	0.5%	0.0%	1.0%	-1.3%	0.3%	0.1%	0.2%	-0.7%
	V_{sSat}	0.5%	0.0%	0.3%	-0.1%	0.1%	0.0%	0.2%	0.1%
	V_pV_{sSat}	0.2%	0.0%	1.0%	-1.3%	0.3%	0.1%	0.0%	0.7%
	k_{Sat}	0.6%	0.1%	**3.6%**	**-4.5%**	0.9%	0.2%	-0.1%	**-2.3%**

Table 1. Errors in derived petrophysical and mechanical parameters associated with the different tested fluid property prediction methods for typical Gulf of Mexico transition zone and supercritical storage reservoir depths. Errors above 1% are shown in red. Errors above 2% are in bold.

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