Supporting Information

Analyses of Interpolant Ion Effects on Smart Water Core Flooding in Carbonate

1. Core flooding modeling

The input of several data is required to build the simulation model. In addition, models need to be selected to calculate the phase properties. For this reason, some relevant data are presented here to support the information given in the manuscript, as follows:

1.1 Gas-Oil relative permeability curve: shown in Figure S1

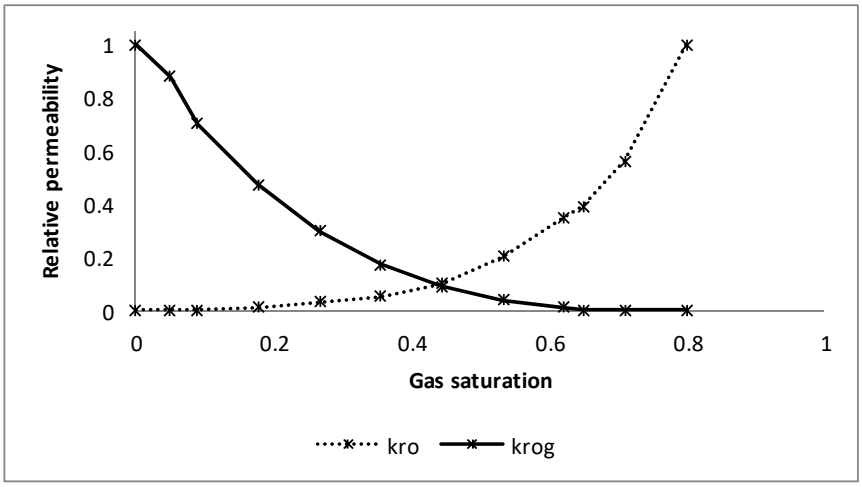

Figure S1. Gas-Oil relative permeability curve

1.2 Three-phase relative permeability: Three-phase relative permeability was predicted by Stone's second model using the previously provided two-phase relative permeability data.

1.3 Reactions considered during simulation

Aqueous reactions:

$CO_2 + H_2O \leftrightarrow H^+ + HCO_3^-$ $\quad log\ K_{eq}(238°F) = -6.50$ **(S1)**

$H^+ + OH^- \leftrightarrow H_2O$ $\quad log\ K_{eq}(238°F) = 12.00$ **(S2)**

$CaSO_4 \leftrightarrow Ca^{2+} + SO_4^{2-}$ $log\ K_{eq}(238°F) = -2.84$ (**S3**)

$MgSO_4 \leftrightarrow SO_4^{2-} + Mg^{2+}$ $log\ K_{eq}(238°F) = -2.67$ (**S4**)

$HSO_4^- \leftrightarrow H^+ + SO_4^{2-}$ $log\ K_{eq}(238°F) = -3.52$ (**S5**)

$KCl \leftrightarrow K^+ + Cl^-$ $log\ K_{eq}(238°F) = 1.14$ (**S6**)

$NaCl \leftrightarrow Na^+ + Cl^-$ $log\ K_{eq}(238°F) = 0.886$ (**S7**)

$CaCl^+ \leftrightarrow Ca^{2+} + Cl^-$ $log\ K_{eq}(238°F) = -0.161$ (**S8**)

$MgCl^+ \leftrightarrow Mg^{2+} + Cl^-$ $log\ K_{eq}(238°F) = -0.483$ (**S9**)

$CaCH3CO^+ \leftrightarrow Ca^{2+} + CH_3COO^-$ $log\ K_{eq}(238°F) = 0.069$ (**S10**)

$MgCH3CO^+ \leftrightarrow Mg^{2+} + CH_3COO^-$ $log\ K_{eq}(238°F) = -1.270$ (**S11**)

Mineral reactions:

$H^+ + Calcite \leftrightarrow Ca^{2+} + HCO_3^-$ $log\ K_{eq}(77°F) = 0.509$ (**S12**)

$2\ H^+ + Dolomite \leftrightarrow Ca^{2+} + Mg^{2+} + 2\ HCO_3^-$ $log\ K_{eq}(77°F) = -0.272$ (**S13**)

Ion exchange reaction:

$0.5\ SO_4^{2-} + CH_3COO\text{-}X \rightarrow CH_3COO^- + 0.5\ SO_4\text{-}X_2$ (**S14**)

1.4 Models for estimating properties: models are summarized in Table S1.

Table S1. Modeling of phase properties in the GEM simulator

	Model
Equation of state (oil and gas)	Peng Robinson[1]
Oil and gas viscosity	Jossi, Stiel and Thodos correlation[2] in association with the Yoon and Thodos[3] and Herning and Zipperer formulation
Aqueous viscosity	Kestin correlation[4]
Aqueous density	Linear method (EquationS15)
CO_2 solubility in water	Henry's law

$$\rho_w = \rho_{w,ref} + (1 + C_w * (P - P_{ref})$$

(S15)

where: P_{ref} is the reference pressure to provide aqueous phase properties values at the beginning of the simulation, ρ_{w_ref} is the density of the aqueous phase at temperature and reference pressure supplied as input data, C_w is the isothermal compressibility for the water component, ρ_w is the density of aqueous phase at desired pressure P.

1.5 Petrophysical properties alteration

A phase resistance factor was considered to allow computing petrophysical properties alteration due to solid deposition and/or mineral precipitation or dissolution. So, a resistance factor was used, as described in Equations S16 and S17.

$$k_n = \frac{k_{n-1}}{r_f}$$

(S16)

where: r_f is the resistance factor calculated by the power law relationship (Equation (), k_n is the permeability at the current time step, and k_{n-1} is the permeability at the previous time step.

$$r_f = \left(\frac{\emptyset_{n-1}}{\emptyset_n}\right)^3$$

(S17)

where: ϕ_n is the fluid porosity at the current time step and ϕ_{n-1} is the fluid porosity at the previous time step.

2. Oil behaviour model

PVT experimental data from Sequeira[5] were used for tuning the EOS. This procedure was necessary before the core flooding simulations. The results of the differential liberation experiment data, regressed using the Winprop simulator developed by CMG, are presented in Figure S2, Figure S3, Figure S4, Figure S5, and Figure S6, highlighting the excellent agreement obtained. They indicate that the properties of the hydrocarbon phases are well modeled by the simulator, estimating values close to the experimental data. A summary of the average deviations obtained for the property values calculated by the model after data regression is presented in Table S2.

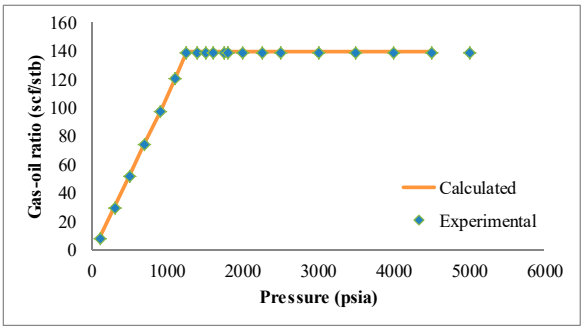

Figure S2. Data regression of differential liberation experiment – Gas-oil ratio

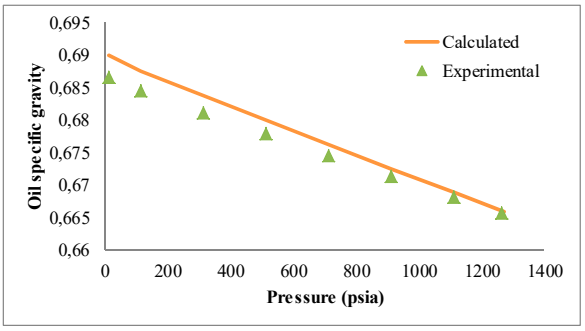

Figure S3. Data regression of differential liberation experiment – Oil-specific gravity

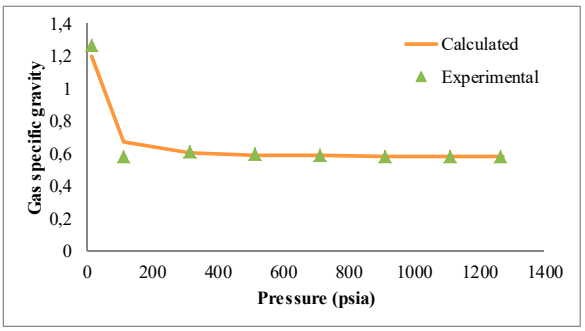

Figure S4. Data regression of differential liberation experiment – Gas specific gravity

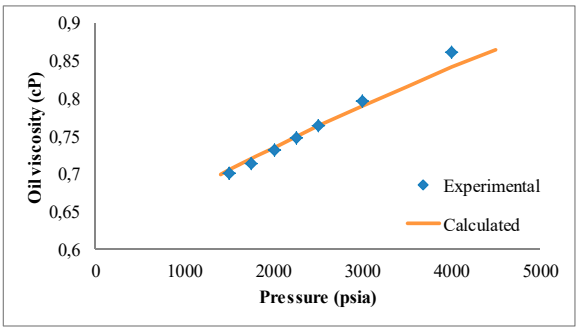

Figure S5. Data regression of differential liberation experiment - Oil viscosity

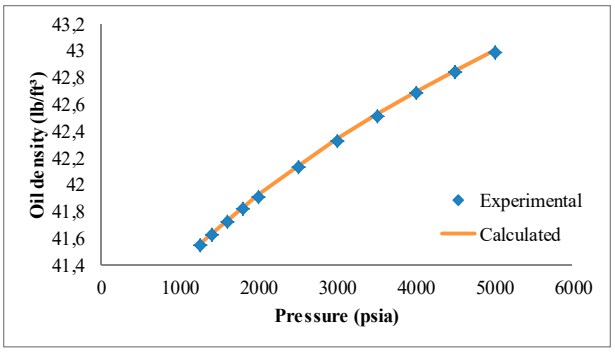

Figure S6. Data regression of constant composition expansion experiment - Oil density

Table S2. The average deviation of the properties estimated by the model after regression of the PVT data

Property	Average deviation (%)
Oil relative volume	0.091
Oil density	0.14
Oil compressibility	0.16
Gas-oil ratio	2.26
Gas compressibility factor	0.65
Gas formation volume factor	0.81
Gas specific gravity	2.94
ºAPI	0.15
Oil viscosity	0.91
Saturation pressure	0.86
Swelling factor	0.48
MMP	3.93

References

(1) Peng, D. Y.; Robinson, D. B. A New Two-Constant Equation of State. *Ind. Eng. Chem. Fundam.* **1976**, *15* (1), 59–64. https://doi.org/10.1021/i160057a011.

(2) Jossi, J. A.; Stiel, L. I.; Thodos, G. The Viscosity of Pure Substances in the Dense Gaseous and Liquid Phases. *AIChE J.* **1962**, *8* (1), 59–63. https://doi.org/10.1002/aic.690080116.

(3) Yoonm, P.; Thodos, G. Viscosity of Nonpolar Gaseous Mixtures at Normal Pressures. *AIChE*

J. **1970**, *16* (2), 300–304. https://doi.org/10.1002/aic.690160225.

(4) Kestin, J.; Khalifa, H. E.; Sookiazian, H.; Wakeham, W. A. Experimental Investigation of Pressure Effect on the Viscosity of Water in the Temperature Range 10-15 Degree C. *Berichte der Bunsengesellschaft/Physical Chem. Chem. Phys.* **1978**, *82* (2), 180–188. https://doi.org/10.1002/bbpc.197800008.

(5) Sequeira, D. S. Compositional Effects on Gas-Oil Interfacial Tension and Miscibility at Reservoir Conditions. Master's Thesis, Louisiana State University, Baton Rouge, LA, USA, 2006.