International Conference on Non-linearities and Upscaling in Porous Media

The Riemann solution for the injection of supercritical carbon dioxide and vapor in porous media

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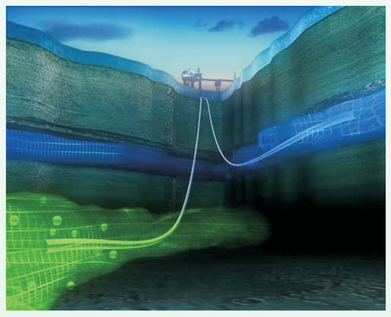
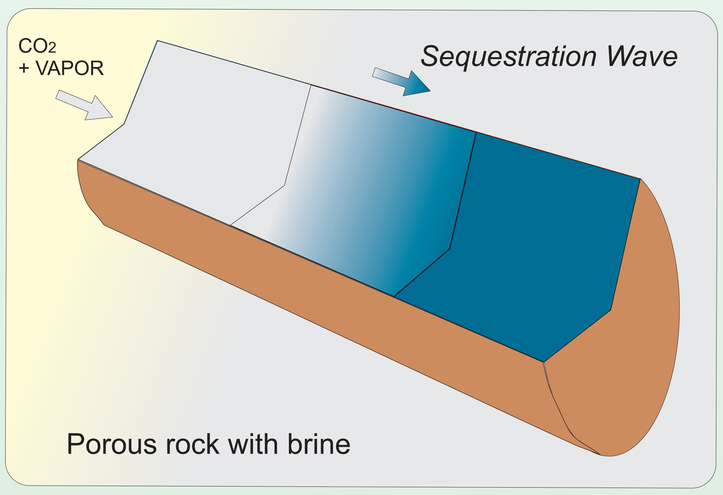


Motivation: ***Study the Riemann Solution for a simplified model of CO_2 Sequestration in brine aquifers. We use a consistent method for calculating the solubility of carbon dioxide in brine. (Electrolyte-NRTL)***



Representation of the model

Summary of variables	
Variable	*Symbol*
Supercritical fluid, aqueous phase saturations	s_σ, s_a
CO_2 and H_2O densities in the supercritical fluid phase	$\rho_{\sigma c}$, $\rho_{\sigma w}$
CO_2 and H_2O densities in the aqueous phase	ρ_{ac}, ρ_{aw}
Total Darcy velocity	u
Supercritical fluid, aqueous phase fractional functions	f_σ, f_a
Supercritical fluid, aqueous phase enthalpies	H_σ, H_a
Rock enthalpy	H_r
Rock porosity	φ
H_20 composition in the supercritical fluid phase	$\psi_{\sigma w}$
CO_2 composition in the aqueous phase	ψ_{ac}

Waves of the compositional flow

Wave Speeds for the Temperature in *x-t* space

Equations of balance

$$\frac{\partial}{\partial t}\varphi\left(\rho_{\sigma c}s_\sigma + \rho_{ac}s_a\right) + \frac{\partial}{\partial x}u\left(\rho_{\sigma c}f_\sigma + \rho_{ac}f_a\right) = 0 \longrightarrow CO_2$$

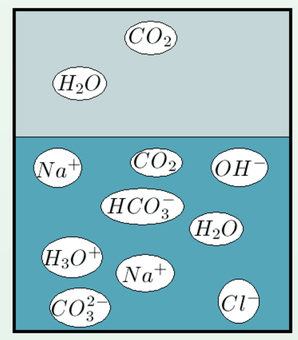
$$\frac{\partial}{\partial t}\varphi\left(\rho_{\sigma w}s_\sigma + \rho_{aw}s_a\right) + \frac{\partial}{\partial x}u\left(\rho_{\sigma w}f_\sigma + \rho_{aw}f_a\right) = 0 \longrightarrow H_20$$

$$\frac{\partial}{\partial t}\varphi\left(\hat{H}_r + H_\sigma s_\sigma + H_a s_a\right) + \frac{\partial}{\partial x}u\left(H_\sigma f_\sigma + H_a f_a\right) = 0 \longrightarrow \text{Energy}$$

Thermodynamical Model and Data

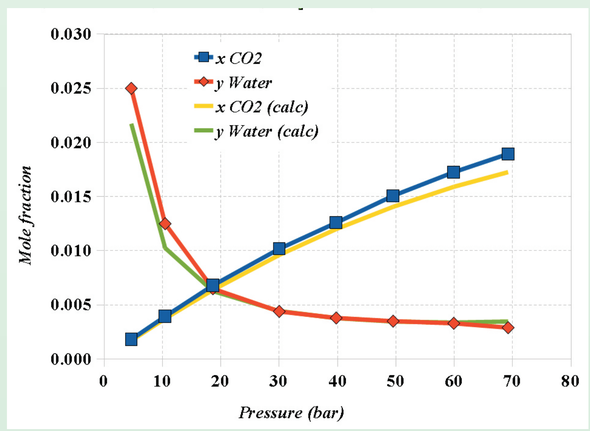
A combination of Electrolyte-NRTL, Redlich-Kwong, and Henry's law are used in the modelling of the supercritical CO_2-H_2O two-phase system.

$$2H_2O \rightleftharpoons H_3O^+ + OH^-$$
$$CO_2 + 2H_2O \rightleftharpoons H_3O^+ + HCO_3^-$$
$$HCO_3^- + H_2O \rightleftharpoons H_3O^+ + CO_3^{2-}$$
$$NaCl_{(s)} \rightleftharpoons Na^+ + Cl^-$$

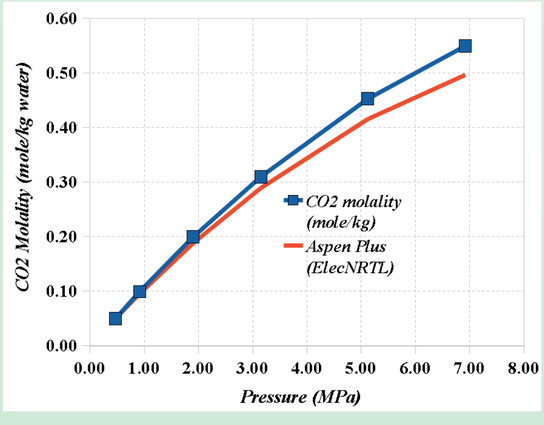


Details of thermodynamical methods used in the calculation of VLE, Densities, and Enthalpy

	Method
Mixture Density	
Liquid	*Electrolyte NRTL- Clarke model*
Vapor	*Redlich-Kwong EOS*
Mixture Enthalpy	
Liquid	*Electrolyte NRTL*
Vapor	*Redlich-Kwong EOS*
VLE parameters	
Liquid activity coefficient	*Electrolyte NRTL*
Vapor fugacity coefficients	*Redlich-Kwong EOS – Henry's law*



Using the Elec-NRTL model of Aspen Plus process simulator in the prediction of P-xy data of CO_2-Water system in 45.08 Celsius.



Experimental CO_2 solubility in the brine solution (molality 3.99) and the Elec-NRTL model results at 40.01 degrees Celsius.

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