Methane-Carbon Dioxide Sorption in Shales Using IAST

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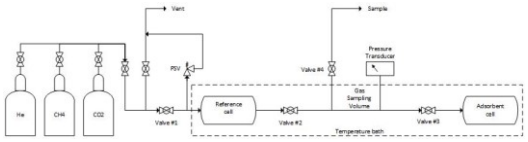
1. Background: Adsorption is a primary storage mechanism in nano-porous gas shales, which are being considered as a low carbon energy source and as a potential carbon sink. Carbon dioxide, owing to it's smaller size, linear shape, and higher surface potential, has a much higher sorption capacity on gas shales compared to methane. Quick and easy prediction of multi-component sorption capacities from single component isotherms is enabled by the Ideal Adsorbed Solution Theory (IAST).

2. Methodology

A generic manometric sorption rig presented in Figure 1 was used in this study (1). Amount adsorbed is measured by injecting known amounts of the adsorptive into the sample cell where the crushed and outgassed shale sample is housed.



Manometric Adsorption Measurement Rig

Ideal Adsorbed Solution Theory was used to predict multi-component sorption capacities at different concentrations of CH4 and CO2. The PyIAST algorithm was used for this purpose (2).

$$f_j = f_j^0 \exp(z_j)\, x_j$$

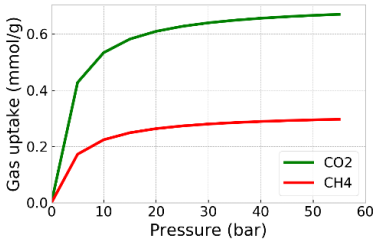
$$\frac{1}{n} = \Sigma_{j=1}^{N} \frac{x_j}{n_j^0}$$

The Langmuir isotherm was used to fit the single component isotherms and the IAST sorption capacities (3).

$$q = \frac{V_L * P}{P_L + P}$$

3. Results (Experimental)

Both CH4 and CO2 isotherms are Type 1 up to 60 bars. The CO2 sorption capacity of shales is nearly 3 times that of CH4 in this case, suggesting that CO2 injection may be technically feasible for CO2 storage and enhanced natural gas recovery.

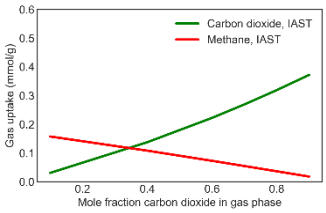


Langmuir Fits for Experimental Values

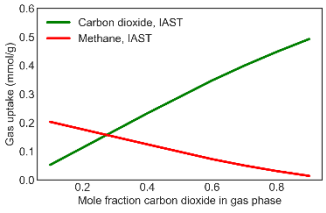
3. Results (IAST Fits)

It is observed that CO2 uptake with respect to loading increases more quickly compared to CH4. This suggests that it might be possible to store nearly 2 or 3 moles of CO2 for every mole of adsorbed CH4 that is displaced.

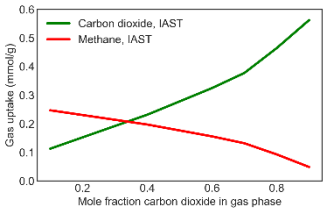
Since the Langmuir pressure of CO2 is lower than that of CH4, the maximum sorption capacity of CO2 is attained at lower pressures compared to CH4. This implies that CO2 stored in the sorbed state would be more stable at lower pressures compared to other CO2 sequestration mechanisms.



IAST Fit 5 Bars



IAST Fit 10 Bars



IAST Fit 60 Bars

5. Conclusion and Further Work

A methodology to predict multi-component sorption from single-component isotherms was demonstrated. We are currently validating predicted IAST sorption capacities against experimental measurements. Once validated, these results may be used to derive insights on various controls on sorption in shales and also to study potential carbon sequestration and enhanced gas recovery technologies.

References
[1] K. Arunachalam, K. Wang, X. Fan, 2019; [2] C.M. Simon, B. Smit, M. Haranczyk, Comput. Phys. Commun. 200 (2016) 364–380; [3] I. Langmuir, J. Am. Chem. Soc. 40 (1918) 1361–1403.