

## A Lattice Fluid Equation of State for Associating CO<sub>2</sub>- Polymer Systems

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We derive a new Lattice-Fluid Equation of State for associating systems by incorporating complex formation in the Sanchez-Lacombe lattice-fluid partition function. We show that the new equation can be used to correlate the solubility of carbon dioxide in several homo and co-polymers over a wide range of temperatures and pressures, and that the extent of swelling in these polymers by CO<sub>2</sub> can be predicted using parameters obtained from the solubility correlation. We also demonstrate that one of the parameters of the equation of state that describes specific interactions between the polymer and carbon dioxide can be quantified using *in situ* Attenuated Total Reflection Fourier Transform Infrared (ATR FTIR) spectroscopy. The calculation of this parameter via NVT molecular dynamics simulation is also described. The new equation of state offers the potential of phase behavior prediction over a wide range of pressures and temperatures using swelling measurements at low pressures.