

# Direct calculation of Henry's law constants from Gibbs ensemble Monte Carlo simulations: Nitrogen, oxygen, carbon dioxide, and methane in ethanol

Ling Zhang and J. Ilja Siepmann\*

*Departments of Chemistry and of Chemical Engineering and Materials Science,  
University of Minnesota, 207 Pleasant Street SE, Minneapolis, Minnesota 55455, USA*

## Abstract

Configurational-bias Monte Carlo simulations in the Gibbs ensemble were used to calculate the Henry's law constants, Ostwald solubilities, and Gibbs free energies of transfer for oxygen, nitrogen, methane, and carbon dioxide in ethanol at 323 and 373 K. These three solubility descriptors can be expressed as functions of mechanical properties that are directly observable in the Gibbs ensemble approach, thereby allowing for very precise determination of the descriptors. Additionally, the Henry's law constants of multiple solutes can be computed from a single simulation. Most of the simulations were carried out for systems containing 1000 solvent and up to 8 solute molecules, and further simulations using either 500 or 2000 solvent molecules point to negligible system size effects. A comparison to experimental data shows that the united-atom version of the transferable potential for phase equilibria (TraPPE) force field yields Henry's law constants that reproduce well the differences between the four solutes and the changes upon increase of the temperature.

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\* Corresponding author: siepmann@chem.umn.edu