Thermodynamic Modeling of Several Aqueous Alkanol Solutions Containing Amino Acids with the Perturbed-Chain Statistical Associated Fluid Theory Equation of State - DTU Orbit (05/12/2018)

Thermodynamic Modeling of Several Aqueous Alkanol Solutions Containing Amino Acids with the Perturbed-Chain Statistical Associated Fluid Theory Equation of State

The perturbed-chain statistical associated fluid theory EoS was applied to model the solubilities of glycine, DL-alanine, L-serine, L-threonine, and L-isoleucine in pure water, pure alcohols (ethanol, l-propanol, and 2-propanol) and in mixed solvent systems. Three pure component nonassociating parameters for the amino acids were fitted to the densities, activity and osmotic coefficients, vapor pressures, and water activity of their aqueous solutions. The solubilities of amino acids in pure and mixed solvent systems were calculated on the basis of the phase equilibrium conditions for a pure solid and a fluid phase. The hypothetical melting properties of each amino acid were fitted, to accurately correlate the solubilities in pure water. Only one temperature independent binary parameter is required for each amino acid/solvent pair. The model can accurately describe the solubility of the amino acids in water, but the correlation for the solubility in pure alcohols was not so satisfactory. The solubility in mixed solvents (ternary systems) was predicted on the basis of the modeling of the solubility in pure solvents, without any additional fitting of the parameters, and the results achieved were reasonable. Fitting the binary parameter for the pair amino acid/alcohol not to the solubility in pure alcohol, but to the solubility in the mixed solvent system, the description of the solubility in the mixed solvent systems was clearly improved and the results were in fair agreement with the experimental data for all mixture compositions. The results showed a global root-mean-square deviation in mole fraction of 0.0032 for correlation and 0.0070 for prediction.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Phase Equilibria and Separation Processes, Center for Energy Resources Engineering
Pages: 5498-5505
Publication date: 2009
Peer-reviewed: Yes

Publication information
Journal: Industrial & Engineering Chemistry Research
Volume: 48
Issue number: 11
ISSN (Print): 0888-5885
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 3.4 SJR 0.978 SNIP 1.203
Web of Science (2017): Impact factor 3.141
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.1 SJR 0.95 SNIP 1.155
Web of Science (2016): Impact factor 2.843
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 2.87 SJR 0.938 SNIP 1.145
Web of Science (2015): Impact factor 2.567
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 2.85 SJR 1.009 SNIP 1.287
Web of Science (2014): Impact factor 2.587
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 2.6 SJR 0.975 SNIP 1.232
Web of Science (2013): Impact factor 2.235
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2