Group Contribution Lattice Fluid Equation of State and the Application to High Pressure Phase Equilibria

<u>알렉산더</u>, 강정원¹, 유기풍* 서강대학교; ¹고려대학교 (kpyoo@sogang.ac.kr*)

The recently proposed multi-fluid nonrandom lattice fluid (MF-NLF) model was used to purpose a method for estimating the equation of state (EOS) parameters using a group contribution (GC) scheme. The group parameters consist of close packed volume and segment number parameters and temperature depended energy interaction parameters. For reliably reproduce equilibrium data near the critical region a new contribution based of Veytsman statistics was introduced into the EOS framework to account for long range density fluctuations, which are know to induce molecular clustering near the critical region. The probability of clustering is modified to be dominant in the critical region. The combination of the GC parameter estimation method and the modified Veytsman contribution were evaluated for various pure and binary equilibrium systems over a wide temperature and pressure range. The results show a remarkable agreement with the presented experimental data, even in temperature and pressure regions near the critical point.