A mult-fluid nonrandom lattice fluid theory for phase equilibria of (intra+ inter) molecular associating systems

<u>신문삼</u>, 신헌용¹, 유기풍², 김화용* 서울대학교; ¹서울산업대학교; ²서강대학교 (hwayongk@snu.ac.kr*)

Intramolecular associating bonds is an important contribution to the overall hydrogen bonding in amphipile systems, especially in systems of colloidal and biological interest. Glycol-ether compounds such as C1E1(2-methoxyethanol), C2E1(2-ethoxyethanol) and C4E1(2-butoxyethanol) form both intramolecular and intermolecular hydrogen bonds. This type of system (polyethoxyalcohols) is of direct interest on alkanol-alkane-ether systems as they involve the same type of interactions, and is of key importance in the study of non-ionic surfactants.

The objective of this study is to present a multi-fluid nonrandom associating lattice model (MALF) for studying fluid systems with both intramolecular and intermolucular associating bonds in alkane + nonionic surfactant systems. Vapor liquid equilibria data for alkane + nonionic surfactant(C1E1, C2E1, C4E1) systems were correlated using intramolecular MALF equation of state. The MALF equation of state for both intramolecular and intermolecular hydrogen bonding for correlating parameters resulted in a better agreement with an experimental data than that for only intermolecular hydrogen bonding.