422f Calculation of Solubility of Hydrogen in Hydrocarbons at High Pressures

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Abstract:

The knowledge of the solubility of hydrogen in hydrocarbons, petroleum fractions and coal liquids is important in petroleum and coal liquid processing. In petroleum refining, hydrogen is added to heavy petroleum fractions to increase their hydrogen to carbon (H/C) ratio and to upgrade their quality through processes such as hydorgenation and hydrotreatment. Addition of hydrogen to heavy petroleum liquids is used for desulfurization and other upgrading processes. In design and operation of equipments related to such processes it is important to know the solubility of hydrogen in the liquid oil. Usually such calculations are made through equations of state (EOS). In this type of modeling specific binary interaction parameters are determined for each fraction. However, for heavy oils that hydrogen is needed for their upgrading all EOS parameters such as critical properties are not known. Even when more advanced equations of state such as Statistical Associating Fluid Theory (SAFT) is used to estimate solubility data specific binary parameters are needed to be determined for each specific system.

It has been shown that regular solution theory of Scatchard-Hildebrand can be used adequately to estimate solubility of light hydrocarbon gases in petroleum fractions under pressure[1]. As under operating conditions hydrogen is in gaseous state, values of molar volumes and solubility parameters provided in the literature are fictitious numbers. In this presentation a simple method is demonstrated to calculate hydrogen solubility in pure hydrocarbons and their mixtures (i.e., petroleum fluids) based on the regular solution theory. Gas phase fugacity can be calculated from an extended virial equation of state. A modified value of solubility parameter is suggested that can be used in the proposed method. In addition a relation is provided for estimation of a fictitious value of fugacity of pure liquid hydrogen at the operating temperature and pressure. The advantage of this technique is that no binary parameter must be determined for a particular hydrocarbon or system and the method is fully predictive. Accuracy of the proposed method is equivalent to that of predictions from an equation of state. However, in the proposed method input parameters such as solubility parameter of liquid molar volume for the solvent can be estimated for heavy hydrocarbons and petroleum fluids with better accuracy than the critical constants needed for an equation of state.

Reference [1] Riazi, M. R., "Characterization and Properties of Petroleum Fractions," ASTM International, Philadelphia, USA, February 2005. (http://www.astm.org/mnl50.htm)