Modeling of POE Lubricants with Two Versions of SAFT Model

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One of the more suitable lubricant kinds for refrigeration systems using HFCs and CO_2 refrigerants are polyol esters (POEs). Most of the POE refrigeration lubricants are based totally or partially on pentaerythritol esters (PEs). Experimental data of vapor pressures [1] of pentaerythritol tetrapentanoate, PEC5, pentaerythritol tetraheptanoate, PEC7, pentaerythritol tetranonanoate, PEC9, and pentaerythritol tetra 2-ethylhexanoate, PEB8, together with saturated liquid densities extrapolated from Tammann-Tait equation [2] were used to tune the parameters for two versions of Statistical Associating Fluid Theory (SAFT) model. The versions considered were SAFT of Huang and Radosz and Perturbed-Chain SAFT (PCSAFT) of Gross and Sadowski.

The parameters obtained for SAFT and PCSAFT versions have shown a linear tendency with the molecular weight for the PEs with linear acid chains, i.e. PEC5, PEC7 and PEC9. It was observed that the quality of fit for both vapor pressure and saturated liquid density is fairly good, such as can be usually expected for a three-parameter equation of state. The vapor pressures were correlated with similar accuracy with both versions, whereas PCSAFT gave the best results for saturated liquid densities. For the compressed densities, SAFT do not describe well the temperature dependence, whereas PCSAFT reproduce quite well the density trend with the temperature. Nevertheless both equations predict a slope $\rho(P)$ higher than the experimental one. Due to the linear behavior of the parameters with the molecular weight, characteristic parameters of other PEs (PEC2, PEC3, PEC4, PEC6, PEC8 and PEC10) were obtained, for which no vapor pressure data are available. PC-SAFT with these parameters predicts quite well the densities at atmospheric pressure.

Using the molecular weight dependence of the characteristic parameters, the densities of three commercial lubricants based in PEs, for which the molecular weights are available, can be predicted with AAD% lower than 1.1% using PC-SAFT. Given that for commercial oils the molecular weight is not always accessible, we propose a method based on the lineality of the kinematic viscosity at 40ºC with the molecular weight for PEs [3]. From the Eychenne and Mouloungui correlation [3] we have determined an effective molecular weight for commercial oils in order to estimate the parameters for SAFT and PCSAFT versions. With this method, densities at atmospheric pressure of commercial lubricants have been well predicted using PC-SAFT.

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