**Thermodynamic Properties Prediction of Oxygenated Components: Using Different Versions of SAFT Equations of State (EOS)**

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Effective design of processes in chemical and petroleum engineering is possible through knowledge of thermophysical characteristics and fluid phase behaviour of multicomponent mixtures. Experimental characterization for broad ranges of temperatures and pressures is time intensive and costly; therefore, predictive thermodynamic models are essential for accurate description of phase behaviour, system optimization, and cost reduction. Indeed, recent advancements in thermodynamic modeling allow today broader estimations from limited experimental data, enhancing both accuracy and efficiency in fluid behavior characterization.

The growing demand for biofuels and biodiesel as substitute energies emphasizes the significance of precise modelling of oxygenated compounds such as fatty acids, triglycerides, and blends with alkanes and other species. These biologically derived molecules have thermodynamic modelling issues that must be addressed in order to enhance optimization of biofuel processes.

This study provides a comparative assessment of various EOS models like SAFT, PC-SAFT, Polar PC-SAFT(P-PCSAFT), and other EOS relevant to oxygenated components in order to establish the most accurate approach for oxygenated components. The models were evaluated based on predictive ability of pure-component and mixture thermodynamic properties, e.g., vapor-liquid equilibrium (VLE), density, and phase behaviour predictions. Compatibility with experimental data was the key aspect for evaluation.

To complete the analysis the retrieval and estimation of EOS parameters was also needed for those chemicals with sparse data available, e.g., glycerol tristearin, tripalmitin, and stearic acid. Accurate parameterization is critical for the applied EOS models as it significantly enhances the precision of thermodynamic property predictions and general model credibility in biofuel-related systems.

Findings suggest that PC-SAFT and related versions of that (P-PCSAFT) provide better accuracy for pure oxygenated components like fatty acids. The study of binary systems, carried out through the Group contribution version of PC-SAFT (GC-PCSAFT) highlights its improved performance upon inclusion of polar and associating interactions.

The results gained are very promising and allow for improved process design of biodiesel production and aid in continuance of attempts at sustainability through enabling more predictable simulations of oxygenated systems of biofuel.

**Keywords:** *Equation of State (EOS), Oxygenated Components, PC-SAFT, SAFT, Parameters, and Thermodynamic Properties*