Isobaric Vapor - Liquid Equilibria of Gasoline Additives Systems At 101.3 kPa

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Abstract
In this study, isobaric vapor-liquid equilibrium of gasoline additives for three ternary systems: "MTBE + Ethanol + 2-Methyl-2-propanol", "Ethanol + 2-Methyl-2-propanol + Octane", and "MTBE + Ethanol + Octane" at 101.3 kPa are studied. Furthermore three binary systems: "ethanol + 2-Methyl-2-propanol", "MTBE + Ethanol", and "MTBE + Octane" at 101.3 kPa have been studied.

The binary system "MTBE + Ethanol" forms minimum boiling azeotrope. The azeotrope data are \( x_{AZ} = 0.955 \) mole fraction and \( T(AZ) = 327.94 \) K. The other ternary systems and the other binary systems do not form azeotrope.

All the literature data used passed successfully the test for thermodynamic consistency using McDermott-Ellis test method.

In this study the calculation of VLE K-values is done by using three methods, the first method uses modified Soave Redlich and Kwong (SRK), modified Peng and Robinson (PR) equations of state for two phases. The second method uses SRK-EOS for vapor phase with (NRTL, UNIQUAC and UNIFAC activity coefficient models) for liquid phase and using PR-EOS for vapor phase with (NRTL, UNIQUAC and UNIFAC activity coefficient models) for liquid phase. The third method uses the Wong- Sandler mixing rules and the PRSV- EOS based on GE of (NRTL and UNIQUAC activity coefficient models).

The non ideality of both vapor and liquid phases for the literature data for the ternary and binary systems have been accounted for predicting VLE K-values using the maximum likelihood principle for parameter estimation which provides a mathematical and computational guarantee of global optimality in parameters estimation.

The Wong- Sandler mixing rules and the PRSV- EOS based on excess Gibbs free energy \( G_E \) of NRTL activity coefficient model give more accurate results for correlation and prediction of the K-values than other methods for the ternary and binary systems which contain asymmetric and polar compounds.

Keywords: VLE, Gasoline Additives, Equations of State, Activity Coefficient Model, Mixing Rule.

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