Prediction of Flash Point Behavior Using UNIFAC and COSMO Method on Liquid Hydrocarbon Mixtures with Addition of Organic Solvents

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The flash point behavior of liquid hydrocarbon mixtures or other organic solvents is critical to safety issues as it provides an indication of the temperature that when the component's vapor will ignite. There are few reports on the flash point of liquid hydrocarbon mixtures with other solvents added despite the importance of its commercial exploitation. This work involves measurement of flash point behaviors when the liquid hydrocarbon mixtures contain different classes of additives. Also, n-decane is used as the surrogate component of the liquid hydrocarbon mixture to simplify the flash point prediction by using the Group Contribution Model (GCM) and COnductor-like Screening MOdel(COSMO) calculation. Analysis of the relation between the mixtures flash point and the non-ideal behavior of the solution is presented by quantifying the properties of the mixtures of non-ideal behavior of real mixtures. This work emphasizes that designing chemical processes is inherently safer when the flash point behavior of liquid hydrocarbon mixtures with specific classes of solvents is presented.