Effect of organic solvent structure on ternary liquid-liquid equilibria of (water + short-chain alcohol + organic solvent) systems

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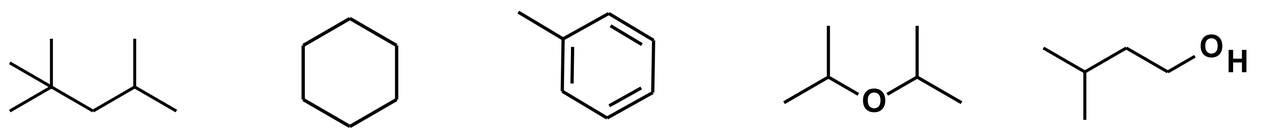
Background And Aim

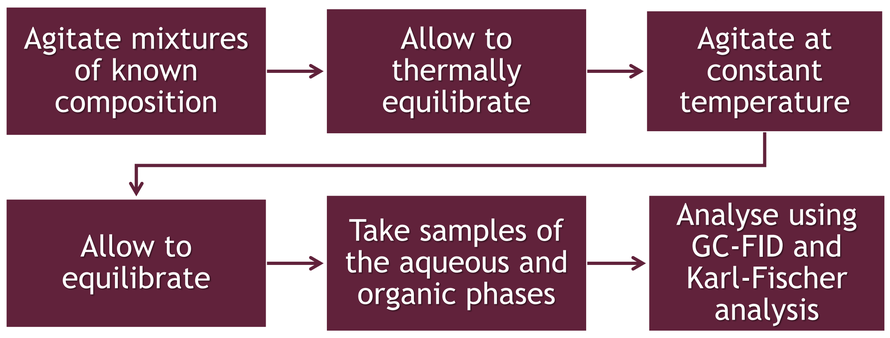
- **Anhydrous short-chain alcohols** are valuable as a fuel alternative
- These alcohols are typically **produced in aqueous water rich streams** in **petrochemical and biological** processes
- LLE data is required for the design and optimisation of **alcohol dehydration** processes

Aim: To evaluate and qualitatively define the effect of organic solvent structure on the liquid-liquid behaviour in ternary systems containing water + normal C2-C4 alcohols + an organic solvent:



Methodology

The method used for this work is based on the method of Swanepoel and Schwarz (2017)



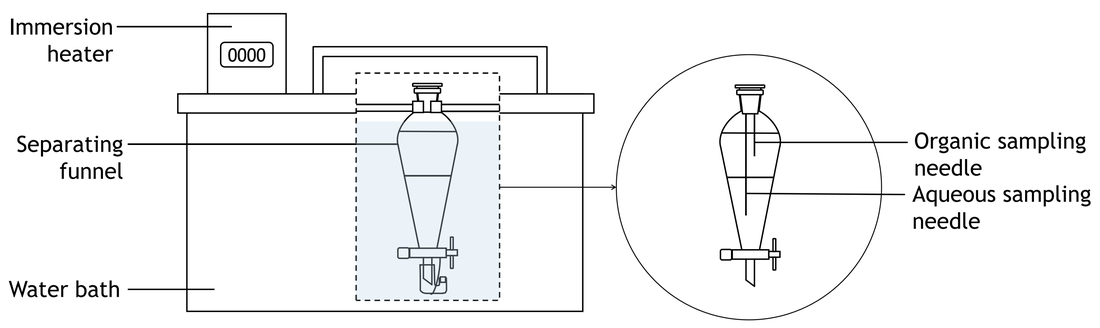


Figure 1: Experimental set-up

Liquid-Liquid Equilibrium Phase Behaviour at 25°C

Water & C2 / C3 alcohols are miscible, forming Treybal Type I regions

Water & C4 alcohol are partially miscible, forming a Treybal Type II region

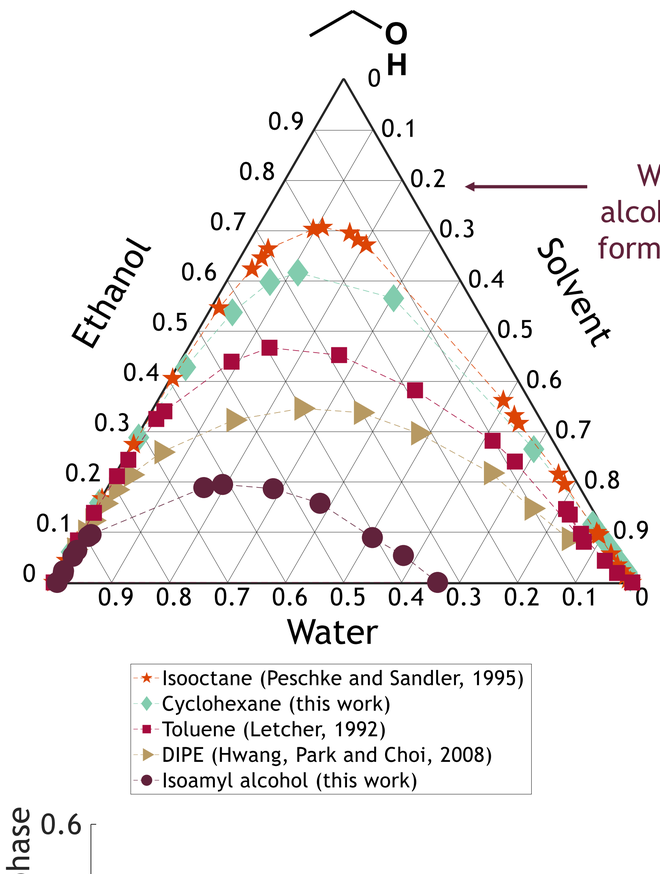


Figure 2: LLE data for (water + ethanol + solvent) systems

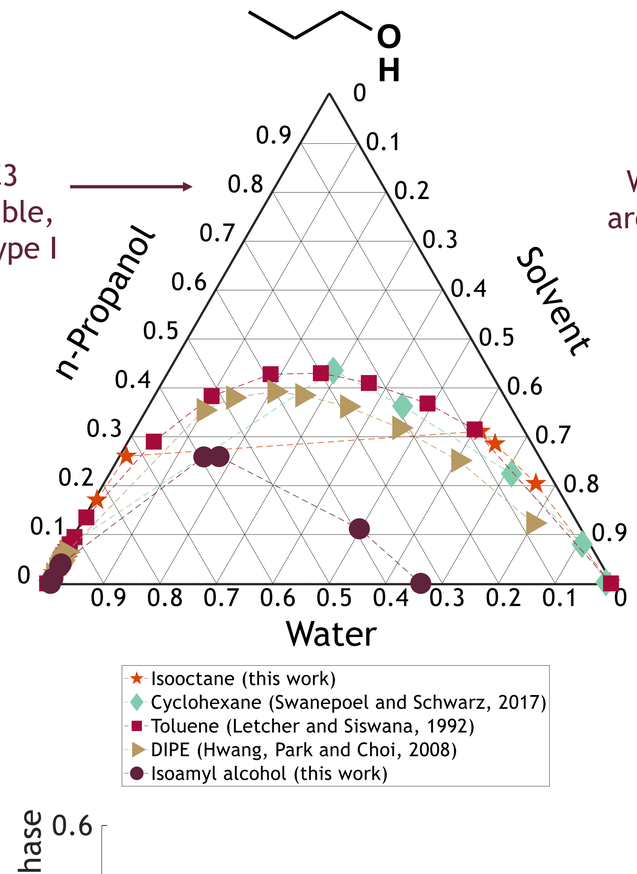


Figure 3: LLE data for (water + n-propanol + solvent) systems

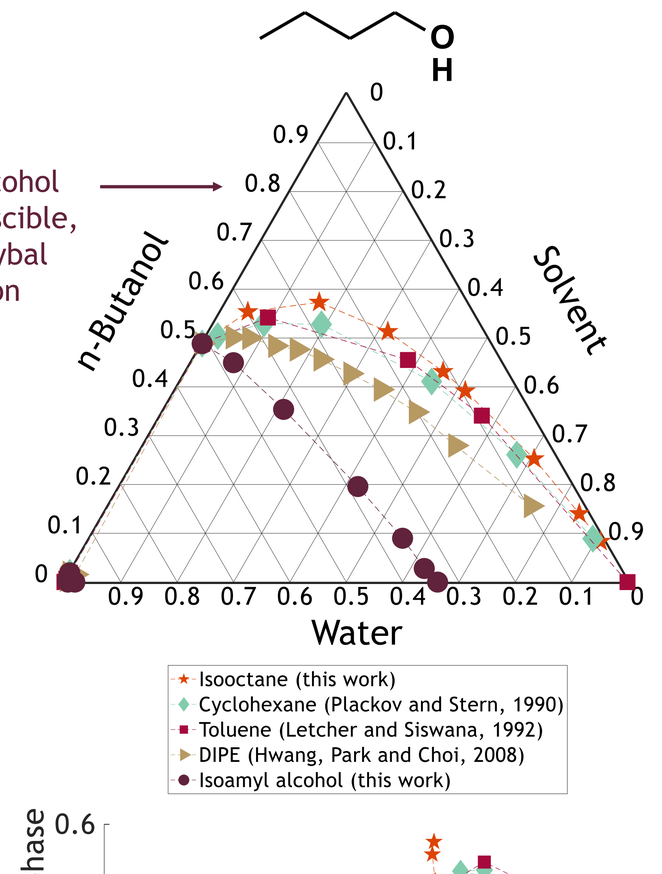


Figure 4: LLE data for (water + n-butanol + solvent) systems

Insights and Future Work

1. Recovery of alcohol to organic phase is highest for oxygenated solvents: DIPE (R-O-R' is a H-bonding acceptor) and isoamyl alcohol (R-OH is a H-bonding acceptor and donor)
2. Less pronounced difference in recovery between solvents for C3 & C4 alcohols due to longer carbon chain alcohols
3. Oxygenated & aromatic solvents experience a decrease in immiscible region size from C4 to C2 alcohols as the alcohol has a higher affinity for water and the solvent with increasing polarity of the alcohol
4. The region size change from C2 to C4 alcohols for aliphatic hydrocarbons is counterintuitive, with the region from smallest to largest: C2>C4>C3
5. For saturated hydrocarbon solvents, there is a lower alcohol recovery, but there is a higher selectivity towards the alcohol as the water content of the organic phase is lower
6. The intermolecular interactions in the ternary systems are temperature dependent and thus an evaluation of these systems at higher temperatures (25°C to 45°C) is recommended

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