Viscosity of glyceline-water mixtures investigated by molecular dynamics simulations

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Deep eutectic solvents (DES) are eutectic mixtures typically formed by a hydrogen bond donor (HBD) and a hydrogen bond acceptor (HBA), with a significant melting point depression relative to the pure isolated components, caused by hydrogen bonding. DES have gained attention as a green and sustainable alternative to conventional organic solvents for having a facile synthesis and purification process, non-flamability, high biodegradability, and low vapor pressure [1]. Two major application areas of DES are metal processing and synthesis media [2]. They have shown to be promising in terms of sustainability and efficiency when preparing recyclable solid sorbents with enhanced sorbant capability, such as metal-organic frameworks [3] and molecular sieves [4] for CO_2 capture, storage, and utilisation purposes. DES have also gained attention recently as green alternatives to traditional solvents for biocatalysis (Figure 1). They can improve substrate supply, conversion, and stability [5] and, unlike organic solvents, DES allow substrates to dissolve without deactivating enzymes and are more sustainable [2, 6].

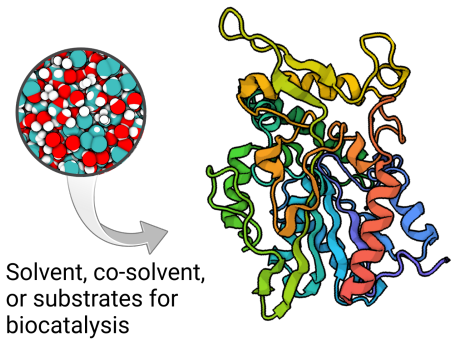

Figure 1: DES have gained attention for biocatalysis, since their properties can be tailored to the required environment by changing the mixture composition and temperature, for example.

Assessing the feasibility of DES for the desired application requires the knowledge of the phase equilibria and activity coefficients, but also thermophysical and transport properties of the components involved. The knowledge of solubility and transport properties in DES strongly impacts process design,

once they are crucial to finding the optimal system and operating conditions. Although DES properties are primarily dependent upon the intermolecular interactions maintained by the components, these properties are challenging to model due to nonideal behavior and complex electrostatics.

Due to the huge number of possible combinations of HBD and HBA, molar ratios, and operating conditions, a large design space is available. Computational modelling is a powerful alternative to experiments for screening of a diverse set of conditions and variables. While thermodynamic modelling is possible for some properties, both static and dynamic properties can be obtained within the same underlying model from tools such as molecular dynamics (MD) simulations [7]. MD can provide fundamental understanding of the physical/chemical mechanisms at atomic scale by simulating systems up to a couple thousand atoms, if appropriate methodologies and force fields are applied.

In this work, we calculate by MD simulations the viscosity of DES aqueous mixture of choline chloride and glycerol (i.e., glyceline - Fig 2). This is a DES used in several reaction types as a solvent or co-solvent [5]. We compare the use of equilibrium and non-equilibrium simulation techniques, evaluate different system compositions, and use a data-integrated approach to provide reproducible simulation data.

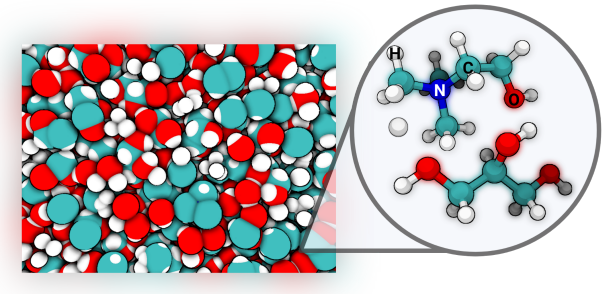

Figure 2: Glyceline is formed by a mixture of choline chloride (HBA) and glycerol (HBD), usually at a 1:2 ratio.

References

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