

Thermodynamic models for physical and thermodynamic properties of Deep Eutectic Solvents: Comprehensive survey two decades after their introduction

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It has been almost two decades since Deep Eutectic Solvents (DESs) were introduced as a novel category of green solvents to the scientific community. In mid-August 2024, a total of 12,730 documents were indexed in the Scopus database on deep eutectic solvents. So, after two decades, it is worthwhile to have an overview of the span of industrial applications for this category of solvents. Are they successfully commercialized yet or still at the research stage in the labs? In addition, it is important to have a survey on the initial research carried out on the fundamentals regarding these green solvents, necessary for any industrial application. This covers knowledge and estimation capabilities of their physical properties. This is the most important fundamental step for investigating any solvent for industrial design and optimization. Therefore, it is vital to have models for estimating a wide range of DES physical properties, from density and viscosity to thermal conductivity. We, at the Des.Solve group, have been working in this field since 2019 to develop different categories of predictive and correlative thermodynamic models, including group and atomic contributions, hybrid machine learning, and semi-empirical models. Our research has led to the development of 20 thermodynamic models for estimating the physical and thermodynamic properties of DEss, covering density, viscosity, surface tension, thermal conductivity, heat capacity, refractive index, and speed of sound. After five years of research, we would like to share the essence of our achievements with the thermodynamic community, from a bird's eye perspective on physical property investigations on deep eutectic solvents. With this experience, it is possible to highlight the future research paths for physical property estimations, emphasizing the current gaps, which are expected to be filled by researchers for better collaborations between academia and the industries.

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