



# High-Precision Estimation of DES Density and Viscosity using Extreme Gradient Boosting: Experimental Insights and Modelling

Krunal J. Suthar<sup>1</sup> · Atir Sakhrelia<sup>2</sup> · Amaan Mansuri<sup>2</sup> · Anaya Patel<sup>2</sup> · Priyank Thakkar<sup>2</sup> · Milind H. Joshipura<sup>3</sup>

Received: 18 December 2024 / Accepted: 4 August 2025

© The Author(s), under exclusive licence to Springer Science+Business Media, LLC, part of Springer Nature 2025

## Abstract

Deep Eutectic Solvents (DESs) have garnered significant interest due to their diverse applications; however, detailed thermophysical data, especially for density and viscosity, are needed to expand their industrial use. This study developed an Extreme Gradient Boosting (XGBoost) model to predict the density and viscosity of DESs. Experimental measurements were conducted on 494 density data points (308–353 K) and 1600 viscosity data points (293.15–323.15 K) from 40 DESs synthesized by varying the molar ratios of three hydrogen bond acceptors and donors. The dataset was used to train an Extreme Gradient Boosting model (XGBoost) for accurate property prediction. The XGBoost model demonstrated high accuracy, with a mean absolute percentage error (MAPE) of 0.16% for density and 1.5% for viscosity. These results indicate that the model is a reliable tool for predicting key thermophysical properties, facilitating the broader application of DESs in various industries.

**Keywords** Machine learning · Boosting · XGBoost · Deep eutectic solvents · Density · Viscosity

## 1 Introduction

The deep eutectic solvent (DES) is a mixture of quaternary salt, commonly known as a hydrogen bond acceptor (HBA), with either a hydrogen bond donor (HBD) or metal halides, forming a low-melting-point liquid. DESs are a promising alternative to the

---

✉ Krunal J. Suthar  
krunal.suthar@upluniversity.ac.in

✉ Milind H. Joshipura  
milind.joshipura@nirmauni.ac.in

<sup>1</sup> Department of Chemical Engineering, Shroff S R Rotary Institute of Chemical Technology, UPL University of Sustainable Technology, Vatariya, Gujarat, India

<sup>2</sup> Department of Computer Engineering, Institute of Technology, Nirma University, Gujarat, India

<sup>3</sup> Department of Chemical Engineering, Institute of Technology, Nirma University, Gujarat, India