Brazilian Journal of Chemical Engineering
https://doi.org/10.1007/s43153-023-00359-2

ORIGINAL PAPER

Experimental measurement and empirical modeling of surface tension of ammonium and phosphonium salt-based DESs

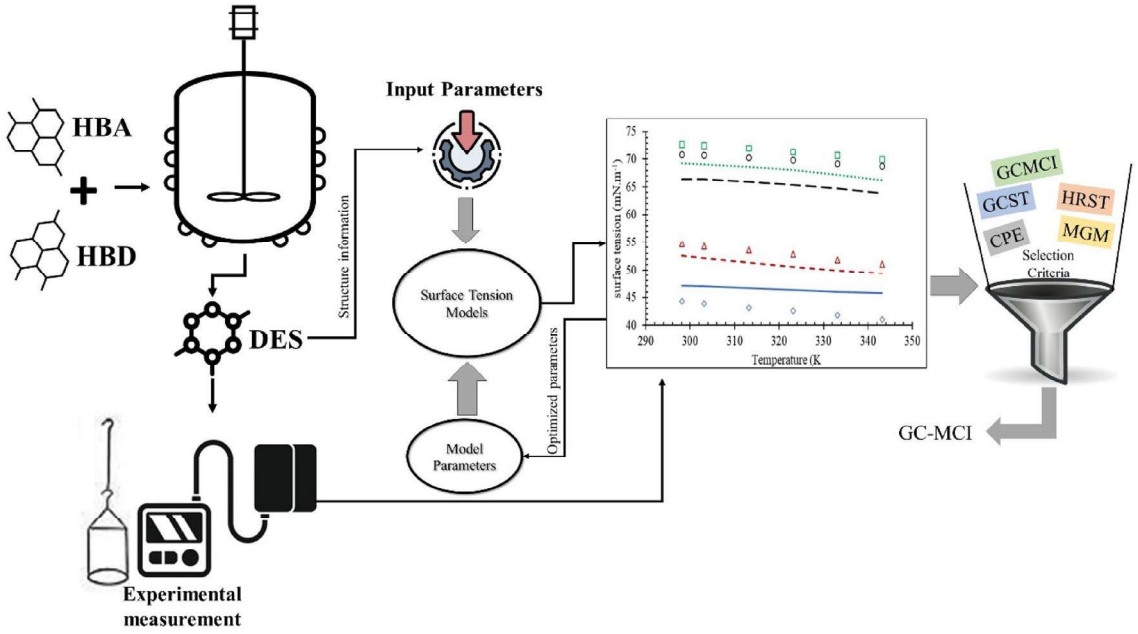
Krunal J. Suthar[1] · **Milind H. Joshipura**[2]

Received: 8 November 2022 / Revised: 25 May 2023 / Accepted: 1 June 2023

Abstract

Deep eutectic solvents (DESs) have been a field of intensive research globally due to their synthetic flexibility and environmentally benign nature. The use of DESs for large-scale industrial applications requires cognizance of their thermophysical properties. Surface tension is a fundamental property essential in design calculations of processes dealing with multiple immiscible interfaces. Herein, we report the 240 data points of experimental surface tension of 45 ammonium and phosphonium salt-based DESs within the temperature range of 298.15 to 343.15 K. Furthermore, a comparative study was carried out on three component-specific and five generalized empirical models. The models were modified, employed, evaluated, and recommended based on statistical assessment and estimation capability for DESs. Nearly 70% of datasets from the synthesized DESs were used to train the proposed model and the rest were used for training purposes. To validate the predictive capability of the proposed model, nearly 100 datapoints of DESs other than those synthesized were employed. The combination of the group contribution method and structural-property relation (GC-MCI) successfully estimated the surface tension of DESs. The overall absolute relative deviation (%OARD) of the component-specific simple linear model and the generalized GC-MCI model resulted in 0.112 and 4.10, respectively.

Graphical abstract



Extended author information available on the last page of the article

Published online: 27 June 2023