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MOLAR VOLUME OF EUTECTIC SOLVENTS AS A FUNCTION OF MOLAR COMPOSITION AND TEMPERATURE

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Abstract:

The conventional Rackett model for predicting liquid molar volume has been modified to cater for the effect of molar composition of the Deep Eutectic Solvents (DES). The experimental molar volume data for a group of commonly used DES has been used for optimizing the improved model. The data involved different molar compositions of each DES. The validation of the new model was performed on another set of DESs. The average relative deviation of the model on the training and validation datasets was approximately 0.1% while the Rackett model gave a relative deviation of more than 1.6%. The modified model deals with variations in DES molar composition and temperature in a more consistent way than the original Rackett model which exhibits monotonic performance degradation as temperature moves away from reference conditions. Having the composition of the DES as a model variable enhances the practical utilization of the predicting model in diverse design and process simulation applications.

Keywords: molar volume; density; physical properties; ionic liquids; eutectic solvents

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