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"Gheorghe Asachi" Technical University of Iasi, Romania

MODELING OF EXCESS MOLAR VOLUME FOR BINARY AND TERNARY MIXTURES OF BENZYL ALCOHOL, n-HEXANOL AND WATER

Iuliana Bîrgăuanu[1], Cătălin Lisa[1], Florin Leon[2], Silvia Curteanu[1], Gabriela Lisa[1]*

[1]"Gheorghe Asachi" Technical University, "Cristofor Simionescu" Faculty of Chemical Engineering and Environmental Protection, 73 Prof. D. Mangeron Blvd., 700050 Iaşi, Romania
[2]"Gheorghe Asachi" Technical University, Faculty of Automatic Control and Computer Engineering, 27 Prof. D. Mangeron Blvd., 700050 Iasi, Romania

Abstract

In this study, the density for binary and ternary mixtures of benzyl alcohol, n-hexanol and water was determined experimentally in a composition range influenced by the miscibility of the components, four temperatures, 293.15, 303.15, 313.15 and 323.15 K, respectively and atmospheric pressure (0.1 MPa). The excess molar volume was calculated in correlation with composition, normalized temperature and refractive index, easily to determine experimentally using a small amount of substance. The 108 data sets were mixed, then randomly divided into 93 for training and 15 for validation stages. For the modelling purpose, artificial neural networks (ANN), with one or two layers of hidden neurons, were built. The best performance was obtained with the ANN neuronal model (4:8:4:1). The standard deviation calculated in the training stage is ± 0.0059 $cm^3 mol^{-1}$, and ± 0.070 $cm^3 mol^{-1}$ in the validation stage. The results obtained with neural models were also compared with those provided by the regression algorithms: k-Nearest Neighbor, Random Forest, Support Vector Machines and Linear Regression. The performance of the Random Forest model with 1000 trees is significantly better than that of the neural model (4:8:4:1). In the validation stage, the correlation coefficient for the Random Forest model was 0.9265, while for the neural model (4:8:4:1) it was 0.6595.

Key words: benzyl alcohol, excess molar volume, n-hexanol, neural models

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* Author to whom all correspondence should be addressed: e-mail: gabriela.lisa@academic.tuiasi.ro