دانشگاه صنعتی خواجه نصیرالدین طوسی
هفدهمین کنفرانس شیمی فیزیک ایران
۲۹ مهرماه ۱ آبان ۱۳۹۳
17th Iranian Physical Chemistry Conference
21-23 October 2014

P481

Prediction of Activity Coefficient at Infinite Dilution for Some Organic Solutes in Ionic Liquid of [BMPYR][TCM] by Using GA-SVM and SR-SVM

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Introduction

The Infinite dilution activity coefficient (γ_{13}^{∞}) of solute is usually used as a parameter to choose solvents for separation. The values of this parameter depends on the type of ionic liquid, so measuring the (γ_{13}^{∞}) is very important. The ionic liquid was used in this study is 1-butyl-1-methyl pyrrolidinium tricyanomethanide,[BMPYR] [TCM] which has quite a high selectivity for the separation of aromatic and aliphatic hydrocarbons. There are some analytical methods for determination of the (γ_{13}^{∞}) [1]. Since, experimental methods are expensive and time consuming, theoretical and computational methodologies such as quantitative structure property relationship QSPR would be helpful in the estimation of the (γ_{13}^{∞}) in ionic liquid of [BMPYR] [TCM].The main aim of the present work is the development of QSPR model by using coupling of genetic algorithm (GA) and (SR) as variables selection and support vector machine(SVM) as modeling tool to predict (γ_{13}^{∞}) some organic compounds in ionic liquid of [BMPYR] [TCM] and the results obtained using SR-SVM and GA-SVM were compared with the experimental values.

Methods

The average experimental (γ_{13}^{∞}) data for 59 solutes at six different temperatures were taken from literature [2]. The chemical structures of the studied 59 solutes were drawn with HYPERCHEM software (ver.7.0) and optimization was done with the AM1 semi empirical method. For each molecule, 1481 molecular descriptors taken from DRAGON software, 21 molecular descriptors from HYPERCHEM and the experimental descriptor of temperature were inserted in the SPSS software. The dataset was randomly split into two sets including training and test sets. The genetic algorithm and stepwise regression (SR) methods were used to select the best descriptors from among the remaining descriptors to construct the model.

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The selected variables by these methods were used as the input of support vector machine (SVM) to predict of (γ_{13}^{∞}) for these compounds. after training and optimization of the (SVM) investigated by the test set.

Result and Discussion

Most significant descriptors were selected by (GA) and (SR) methods are 10 and 12 respectively. The quality of SVM for regression depends on several parameters including: kernel type k, which determines the sample distribution in the mapping space and its corresponding parameters γ, capacity parameter c, ε, and ε-insensitive loss function. Three parameters were optimized in a systematic grid search way and the final optimal model was determined as c=48.6, 900, γ =0.071, 0.005 ε = 0.86,0.0001, for GA-SVM and SR-SVM respectively. The predicted GA-SVM and SR-SVM of the (γ_{13}^{∞}) of the test sets are plotted versus their experimental values in figures1, 2 and their residuals in figures3, 4 respectively.

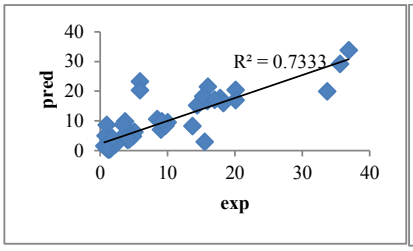

Fig1.plot of the predicted (γ_{13}^{∞}) versus experimental values by GA-SVM

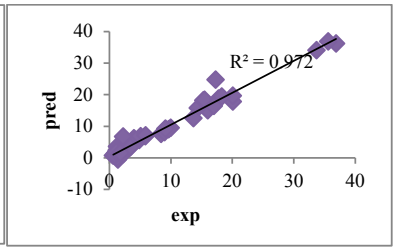

Fig2.plot of the predicted (γ_{13}^{∞}) versus experimental values by SR-SVM.

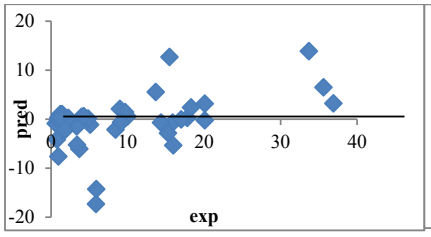

Fig3.plot of the residuals versus experimental Values of (γ_{13}^{∞}) by GA-SVM

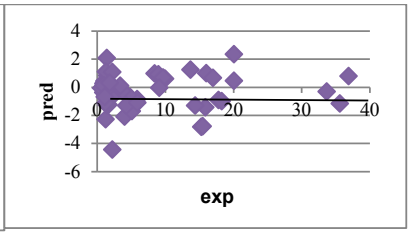

Fig 4.plot of the residuals versus experimental values of (γ_{13}^{∞}) by SR-SVM

Conclusions

In the present work, the SR-SVM model was successfully used to predict the (γ_{13}^{∞}) of organic compounds. the results obtained showed that most of the predicted values of (γ_{13}^{∞}) agreed with the experimental values satisfactory, with the predicted errors within the range of the experimental error.

References

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[2] U.Domanska, E.V. Lukoshku, J. Chem. Thermodynamics 66 (2013) 144-150