

Environmental Chemical Sensing Using Quartz Microbalance Sensor Arrays: Application of Multicomponent Analysis Techniques

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An array of piezoelectric quartz crystals was applied for the detection of volatile organic compounds such as hydrocarbons, chlorinated compounds and alcohols. Steady-state frequency shifts have been used as input parameters for the multicomponent analysis algorithms. The coating materials chosen were stable polymers, i.e., side-chain-modified polysiloxanes. To perform multicomponent analysis, we comparatively employed commercially available partial least-squares regression software (PLS) and artificial neural networks (ANN). The neural network designed for this application was small in order to avoid overfitting. Critical comparison of the performance of the tested algorithms with respect to the ability of prediction and the time required for model building shows that the neural network yields significantly better results than PLS for the analysis of mixtures of more than two compounds. For low-dimensional problems such as the analysis of binary mixtures of dissimilar hydrocarbons, the results achieved here clearly show that there is no improvement in the prediction capability using ANN evaluation. The complexity of the problems is predicted by methods of exploratory data analysis and the estimations are verified by the performance of the algorithms used in our work.

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