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Method for determining the parameters ΔH_s and ΔS, to simulate the retention time in gas chromatography for Malathion, Fenitrothion and Clorpirifos

Cristian Camilo Ortiz Yara[1], Olga Lucia Ramos Sandoval[1], Dario Amaya Hurtado[1]

[1]Universidad Militar Nueva Granada, Facultad de Ingeniería en Mecatrónica, Bogotá, Colombia; Grupo de Aplicaciones Virtuales – GAV.

Abstract: Gas chromatography (GC), is consider as one of the best analytical techniques due to their speed and effectiveness in the identification and quantification of pesticides in food. These parameters depend on the type of column, the pressure and temperature programmed inside the system. The relationship between these is not linear. Due to this, it is requires the development of a model for predicting the retention time (RT), with the aim of optimizing the process and thus spend fewer resources in the trial. To carry out this prediction, it was determined the parameters ΔH_s and ΔS . It was taken in account the results obtained in other studies and they were adjusted to the predictive model. It were developed the parameters of the predictive model in a DB-5 column. Parameters were obtained (ΔH_s [KJ / mol]; ΔS [J / mol K]) with values (-106, -170) (-72.7, -100) and (-107, 171.1) for Malathion, Fenitrothion and Clorpirifos respectively. It was found that these values depend on the polarity of the compound given by it is chemical structure.
Keywords– Chemical pesticide, Liquid chromatography, Retention time.

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