

INVESTIGATION OF PARTITIONING OF  
AROMATICS BETWEEN ACETONITRILE AND NON  
POLAR SOLVENTS

By

K.V.G.M. De Silva.



PERMANENT REFERENCE

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UNIVERSITY OF COLOMBO, SRI LANKA.

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## ABSTRACT

Investigation of partition coefficients of selected polar aromatic compounds between acetonitrile and hexane, which were in simulated polycyclic aromatic hydrocarbon (PAH) samples, were initially performed in this project.

A mixture of PAHs containing naphthalene, 1,4-dimethyl naphthalene, acenaphthene, fluorene, ananthracene, anthraldehyde dissolved in acetonitrile were extracted with hexane. This was repeated for several aliquots of simulated samples with variable volumes of hexane with the intention of working out partition coefficients ( $K_d$ ). Chrysene and benzo(a)pyrene were separately analyzed for this purpose using a fluorimeter.

It has been found that the values of partition coefficients ( $K_d$ ) of 1,4-naphthaquinone, acenaphthene, fluorine, anthracene, anthraldehyde, benzo(a)pyrene and chrysene between acetonitrile and hexane were 0.88, 0.08, 0.68, 0.91, 1.54, 2.19, and 3.92 respectively.

Acetonitrile was utilized as a solvent for the purpose of extracting aromatics from diesel in this project. Subsequent analysis of this extract using the GC/MS revealed that the hydrocarbons present in diesel were also extracted together with aromatics and PAHs. When the same extracted aliquot was analyzed in GC/MS after washing it with hexane, it was found that almost all of the hydrocarbons extracted into the hexane layer leaving aromatic and PAHs in the acetonitrile layer.

Aromatic compounds such as methyl phenol, dimethyl phenol, dibenzothiophene and PAHs such as naphthalene, methyl naphthalene, dimethyl naphthalene, 1'1'-biphenyl-4-methyl, trimethyl naphthalene, 9H fluorene-2-methyl, anthracene, methyl anthracene, 9H carbosol-2-methyl were identified in the diesel analyzed in this project. It was conspicuous further from the results in GC/MS analysis that the methyl naphthalene, dimethyl naphthalene incorporated in diesel significantly with compare to the rest of the PAHs present in the diesel.

It was demonstrated in this project that the amount of PAHs present in diesel can be reduced utilizing continuous extraction process. It was conspicuous in this project that the extractability of PAHs into acetonitrile enhanced with time. The latter information was gathered after analyzing each diesel extract in acetonitrile by using HPLC with a fluorescence detector. Based on the continuous extraction results it was found that 2.63% of dimethyl naphthalene, 0.08% of methyl naphthalene, 0.03% of naphthalene and 0.04% of anthracene were present in diesel. In addition 1'1-biphenyl-4-methyl, naphthalene-1,4,6-trimethyl, 9H fluorene-2-methyl, dibenzothiophene, anthracene-2-methyl, 9H carbosol-2-methyl were found in diesel. They couldn't be quantified due to lack of standards and their coelution during the chromatographic analysis.