Using Computational Chemistry to Determine the Fate of Organic Pollutants - Physico-Chemical Properties of PFOA and PFAAs

By Mauricio Centeno

Supervisor: Nelaine Mora-Diez
Committee Members: Bruno Cinel & Mila Kwiatkowska

Perflourooctanoic acid (PFOA) and other perfluorinated alkyl acids (PFAAs) have been found distributed across soil, air and groundwater around the world. These compounds have been widely used as polymerization precursors of fluoropolymers such as PTFE (polytetrafluoroethylene, or Teflon©). PFAAs and fluoropolymers are used as water and oil repellent in carpets, leathers, fabrics, wax papers (food packaging), floor waxes, and in fire-fighting foams. Since these chemicals are toxic, possibly carcinogenic, and persistent in the environment, there is growing interest on determining the mechanisms of transportation and distribution of these contaminants through the environment. Two of the most important physico-chemical properties to elucidate the pattern that these contaminants follow are the acid dissociation constant (pK_a) and the partition coefficient in octanol:water (K_{ow}). Efforts have been made to obtain valid results but no figures have been accepted as irrefutable. Using Computational Chemistry, this study pretends to provide the missing data by performing the theoretical determination of pK_a and K_{ow} for the series of PFAAs isomers with 8 carbons (39 molecules, including the linear PFOA).