

MECHANISMS OF SLOW SORPTION OF THE NEUTRAL AND CHARGED FORMS OF PENTACHLOROPHENOL ON SOIL

I. P. DiVincenzo and D. L. Sparks

Department of Plant and Soil Sciences, University of Delaware,
Newark, Delaware

Ionizable organic chemicals present a unique environmental concern due to the extensive physicochemical differences between the two species. In addition, they present us with an opportunity to explore differences in soil sorption mechanisms for the two molecular species. Pentachlorophenol (PCP) has a pK_a (4.75) within an environmentally relevant pH range. Therefore it can exist in either the charged (ionized) or neutral (protonated) form within the environment.

Chemicals with reactive functional groups are more prone to a slow specific reaction with the surface that could eventually result in the formation of a bound residue. Intraorganic matter and intraparticle diffusion are two postulated mechanisms for the slow sorption stage of nonionized hydrophobic organic chemicals. In terms of environmental health it is extremely important to distinguish between these two types of mechanisms. An organic contaminant that is truly irreversibly bound to the soil may not be a threat to ground or surface waters. However, if the pollutant is slowly diffusing outward it remains a constant threat to our water resources.

Our studies have shown the slow sorption of the ionized form of PCP on soil is hindered when compared to the neutral form. The slow sorption stage is much more pronounced for the neutral form. In addition, the neutral form remains available to slowly diffuse outward. On the contrary, the ionized form is more resistant to removal even after extended desorption times. Differences in sorption isotherms also suggest that there are different sorption mechanisms for the two species of PCP.

To help ascertain the mechanism, temperature, competitive compound, and humic acid studies were carried out over a range of pH values. The competitive studies explored the sorption of PCP both in the absence and presence of a competing organic compound. Dissolved humic acids have relatively small dimensions and intrasorbent diffusion should be of little importance (1, 2). Any resistance to desorption (hysteresis) found with increasing sorption time will be the result of specific surface reactions. Sorption-desorption and fourier transform infrared spectroscopy (FTIR) studies using humic acids, were carried out to help elucidate the mechanistic differences between the species.

- (1) McCarthy, J. F.; Jimenez, B. D. *Environ. Sci. Technol.* **1985**, 19, 1072-1076.
- (2) Carter, C. W.; Suffet, I. H. *Environ. Sci. Technol.* **1982**, 16, 735-740.