A rapid method for the estimation of the environmental parameters octanol/water partition coefficient, soil sorption constant, water to air ratio, and water solubility

By


Contents

I. Introduction ...................................... 17
II. Experimental ..................................... 19
   a) HPLC system . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 19
   b) Water solubilities (WS) ............................. 20
   c) Soil sorption constants (Koc) and octanol/water partition coefficients (Kow) ............................... 20
III. Results and discussion . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 21
   a) Reverse phase high-performance liquid chromatography (RP-HPLC) and soil sorption constants (Koc) .............. 21
   b) Reverse phase high performance liquid chromatography (RP-HPLC) and octanol water partition coefficient (Kow), bioconcentration factor (BCF). .............................. 23
   c) Reverse phase high-performance liquid chromatography (RP-HPLC) and water solubility ....................... 24
   d) Estimation of water-to-air ratio (Kw) ................... 24
   e) Soil volatility ................................... 26
Summary ........................................... 26
References . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 26

I. Introduction

The passage of the Toxic Substances Control Act (TSCA) heavily impacts on both industry and government. No longer is environmental hazard assessment limited to those in the agricultural fields. The implication of TSCA is that all classes of chemicals must be assessed as to their environmental hazard. Yet to

*The Dow Chemical Company, Agricultural Products Dept., 9001 Building, Midland, MI 48640.

© 1983 by Springer-Verlag New York Inc.
Residue Reviews, Volume 85.
obtain the data using methodologies such as those called for by the Federal Insecticide, Fungicide, and Rodenticide Act (FIFRA) would be impractical and prohibitive from the aspects of both time and cost. Therefore, the benefits of methodology that allow for early estimation of environmental properties for large numbers of compounds simultaneously and in a rapid and economical manner are readily apparent.

A method that can accomplish this is based upon reverse phase high performance liquid chromatography (RP-HPLC). Partitioning of a chemical between organic and aqueous phases of an RP-HPLC column parallels partitioning that takes place between various phases of the environment. A chemical placed in soil, for example, will partition between the soil organic material and soil water and between the soil water and soil air (Fig. 1). The primary physical properties of the chemical which determine how a chemical will become distributed are its hydrophobic character and its vapor pressure. The degree of hydrophobicity is related to the tendency of a chemical to migrate to nonpolar media in the environment.

Physical environmental partitioning processes can be defined in terms of equilibrium expressions between compartments which are summarized in Table I. Partition coefficients between water and air ($K_{wa}$), water and soil ($K_{oc}$), and water and biota ($BCF$), as well as water and octanol ($K_{ow}$) do, to some extent, express the hydrophobic character of a chemical and can therefore be related to behavior on an RP-HPLC column.

Typically, these columns have a stationary nonpolar coating of a long-chain, C$_{18}$, hydrocarbon bonded to an inert support. Chemicals which are more soluble in the organic stationary phase, more hydrophobic, will exhibit longer retention times which can be correlated with the different partition coefficients. McCall

![Fig. 1. Conceptual model of soil system.](image-url)