Appendix P

Earthworm Fugacity Estimation

The T-REX model (USEPA 2008) is useful for assessing exposures of terrestrial animals to pesticide residues on foliar surfaces of crops and seeds. The model cannot be used to assess pesticide exposures to terrestrial animals resulting from consumption of earthworms contaminated with pesticide mass present in the soil of the application site. In order to explore the potential exposures of mammals and birds to pesticides in the soil and earthworms on the treatment site, a simple fugacity approach can be employed to estimate concentrations of the pesticide of interest earthworms.

Fugacity is most often regarded as the "escaping tendency" of a chemical from a particular phase. Fugacity (F) has units of pressure, generally pascals (Pa), and can be related to phase concentrations. For any particular environmental phase (*e.g.*, water, soil, air, or biota) there is a corresponding "fugacity capacity" with units of mol/m^3-Pa and is denoted by Z. The relationship between fugacity, fugacity capacity and chemical concentration (C) is defined by Equation 1.

Equation 1. $C = Z * F$

Fugacity capacities for a given chemical are calculated for the phases of interest as part of the exposure point estimation methodology (Mackay and Paterson 1981). The following calculations of fugacity capacities for soil (Z_S) and earthworms (Z_E) (Equations 2 and 3, respectively) require several chemical-specific parameters and assumptions of system temperature (25^{o}C) and steady state equilibrium. Parameter values relevant to Equations 2 and 3 are defined in Table 1.

Equation 2. $Z_S = \frac{K_d * \rho_S}{H}$

Equation 3. $Z_E = \frac{L * K_{OW}}{H}$

Fugacity capacities for a given chemical are calculated for the phases of interest as part of the exposure point concentration estimation methodology. By definition, the ratio between Z values of different phases (compartments) equals the partitioning coefficient (*e.g.*, Equation 4).

Equation 4. $\frac{Z_{oc\,\tan ol}}{Z_{water}} = K_{OW}$

In this approach, it is assumed that a pesticide partitions between the soil, the (pore) water and the air contained within the soil of the treatment site. It is assumed that earthworms dwelling within the soil are exposed to a pesticide via ingestion of contaminated soil. The concentration of a pesticide in earthworm tissues can be calculated according to Equation 5 (see Table 1 for parameter definitions).

Equation 5. $C_E = C_S * \left(\frac{Z_E}{Z_S} \right)$

Table 1. Summary of parameters relevant to earthworm fugacity model.

Symbol	Definition	Units
C_E	Chemical concentration in earthworm tissue	mol/m^3
C_E'	Chemical concentration in earthworm tissue	g/kg
C_S	Chemical concentration in soil	mol/m^3
H	Henry's Law constant	m^3-Pa/mol
K_d	Soil partitioning coefficient	cm^3/g
K_{OW}	Octanol to water partition coefficient	none
L	Lipid fraction of earthworm	none
MW	molecular weight of chemical	g/mol
Z_E	Fugacity capacity of pesticide in earthworms	mol/m^3-Pa
Z_S	Fugacity capacity of pesticide in soil	mol/m^3-Pa
ρ_E	density of earthworm	kg/m^3
ρ_S	Bulk density of soil	g/cm^3

Equation 5 can be redefined using Equations 2 and 3 as follows in Equation 6. Equation 6 is used to calculate the concentration of a pesticide in earthworms inhabiting the soil of treatment sites.

$$\textit{Equation}\quad 6.\quad C_E = \frac{C_S * L * K_{ow}}{K_d * \rho_s}$$

C_S is intended to be representative of the steady-state concentrations of the pesticide of interest in soil. This value is calculated using PRZM. Kd and Kow are chemical-specific parameters. Kd should be consistent with the value input into PRZM. ρ_S is dependant upon the soil properties of the selected PRZM scenario used to derive C_S. L is based on the lipid content of earthworms, which was assumed to be 0.01 (Cobb et al. 1995). The resulting C_E value is in units of mol/m^3. This value is converted to units of g/kg using Equation 7. The density of the earthworm (ρ_E) is assumed to be 1000 kg/m^3 (equivalent to density of water).

$$\textit{Equation}\ 7.\quad C_E' = \frac{C_E * MW}{\rho_E}$$

References:

Cobb, G.P., E.H. Hol, P.W. Allen, J.A Gagne, R.J. Kendall. 1995. Uptake, metabolism, and toxicity of terbufos in the earthworm (*Lumbricus terrestris*) exposed to COUNTER-15G in artificial soils. Environ. Toxicol. Chem. 14(2):279-285.

Mackay, D. and S. Paterson. 1981. Calculating fugacity. Environ. Sci. Technol. 15: 1006-1014.

USEPA. 2008. User's Guide: T-REX Version 1.4.1 (Terrestrial Residue Exposure model). United States Environmental Protection Agency. Environmental Fate and Effects Division.