2.3. General chemical properties related to environmental fate

NB: where the stored parameter differs significantly from the information stated below this will be described in the accompanying text field.

Parameter	Explanation
Solubility in water: mg/l	The mass of a given substance (the solute) that can dissolve in a given volume of water. Value reported is at 20°C. Note for some chemicals solubility may be pH sensitive.
Solubility in organic solvents: mg/l	The mass of a given substance (the solute) that can dissolve in a given volume of solvent. Value reported is at 20°C. Note for some chemicals solubility may be pH sensitive.
Melting point: °C, at 1 atmosphere pressure	The temperature at which the given substance changes its physical state from solid to liquid.
Boiling point: °C, at 1 atmosphere pressure	The temperature at which the vapour pressure of the substance in its liquid state equals the environmental pressure surrounding the liquid i.e. it boils
Degradation temperature: °C, at 1 atmosphere pressure	The temperature at which the substance is no longer stable and begins to break down.
Flash point: °C	The flash point of a flammable substance is the lowest temperature at which it can form an ignitable mixture in air.
Octanol-water partition coefficient as LogP:	LogP is the logarithm (base-10) of the partition coefficient between n-octanol and water. It is used in environmental fate studies and large values (+4 or higher) are regarded as an indicator that a substance will bio-accumulate. For some substances LogP will be very sensitive to pH.
Bulk density/Specific gravity:	Parameter given depends on the physical state (solid or liquid) of the chemical. Solids - Bulk Density is the weight of the chemical per unit volume. Liquids - Specific Gravity is the ratio of the density of the chemical to the density of water.
Dissociation constant pKa:	Strengths of acids and bases can be indicated on a common scale at 25°C. Defined as the negative logarithm of the acidity constant Ka. The lower the pKa the stronger the acid. For example acetic acid has a pKa of 4.75 whilst sulphuric acid has a pKa of -3.0. pKa is used here as an indicator of the potential of a compound to form ions in water. Many chemicals are either permanently ionic or will change ionic state somewhere in the range of the pH of environmental soils and water. Knowing the ionic sate of a chemical provides important information on its potential mobility and persistence in the environment.
Vapour pressure: mPa	The pressure at which a liquid is in equilibrium with its vapour at 25°C. It is a measure of the tendency of a material to vaporise. The higher the vapour pressure the greater the potential.

Parameter	Explanation
Henry's law constant Dimensional / Dimensionless:	A Gas Law states that the amount of gas absorbed by a given volume of liquid at a given temperature is directly proportional to the partial pressure of that gas in equilibrium with that liquid. As such it provides an indication of the preference of a chemical for air relative to water i.e. its volatility. Henry's Law Constant is usually quoted in Pa.m3/mol or in a dimensionless form at 20°C.
Refractive index	This is an optical term and is a dimensionless number that describes how light, or any other radiation, propagates through that medium.
Surface tension mN/m	The tendency of the surface of to resist an external force.
Max UV-Vis absorption L/mol cm	Different compounds may have very different absorption maxima and intensities. The wavelength of maximum absorbance is a characteristic value and so can be used for identification purposes.
General biodegradability:	Short text giving comment on the general biodegradability of the pesticide in the environment.
DT50 Soil	DT50 is the time required for the chemical concentration under defined conditions to decline to 50% of the amount at application. In many cases chemicals show "half-life" behaviour, in which subsequent concentrations continue to decline by 50% in the same amount of time. In such cases several or more four half-lives (in which the concentration declines to 1/8 or 1/16, e.g.) are a measure of the persistence on the chemical.
Soil degradation DT50 Typical/ Laboratory/ Field: (days)	DT50 in a field or laboratory soil sample. Three parameters are given. Typically data is derived from laboratory studies, but where the substance is persistent in soil under laboratory conditions, field studies may be carried out. 'Typical values' quoted are those given in the general literature and are often a mean of all studies field and laboratory.

Notes:

(i) ***Similar data is given for the DT90 i.e. the time in days for the pesticide to decline by 90%.***
(ii) ***Where the pesticide has been assessed by the EU and where data is available the DT50 used in the modelled risk assessment is also provided.***
(iii) ***More detailed data where DT50 is available by soil type, pH, organic carbon for both lab and field studies is available in the off-line MS Access database available under a licence agreement.***

Parameter	Explanation
Soil sorption Koc / Kfoc	Sorption coefficient data is a measure of the tendency of a chemical to bind to soils, corrected for soil organic carbon content. Values can vary substantially, depending on soil type, soil pH, the acid-base properties of the pesticide and the type of organic matter in the soil. Where data is available both the linear (koc) and non-linear (kfoc) parameters are given. Three summary parameters are given for Kfoc and two for Koc.

Note:

(i) ***More detailed data where Koc/Kfoc plus related parameters are available by soil type (sand/silt/clay distribution as well as structure type), pH, organic carbon is available in the off-line MS Access database available under a licence agreement.***

Parameter	Explanation
Dissipation rate RL50 on plant matrix:	The RL50 (Residual Level) is the rate in days for which the pesticide declines by 50% on the surface of the specified plant matrix (leaves, fruit, roots, seeds, grain etc.).

<table>
<tr><th>Parameter</th><th>Explanation</th></tr>
<tr><td>Dissipation rate RL50 on and in plant matrix:</td><td>The RL50 (Residual Level) is the rate in days for which the pesticide declines by 50% on and in the specified plant matrix (leaves, fruit, roots, seeds, grain etc.).</td></tr>
<tr><td colspan="2">Note:
(ii) More detailed data where DT50 is available by crop/plant/tree type and matrix (fruit, leaves, foliage, rind, peel, tuber) studies is available in the off-line MS Access database available under a licence agreement.</td></tr>
<tr><td>Aqueous photolysis DT50 (days) at 20^{o}C pH 7:</td><td>Photochemical processes may be important in determining the fate of organic pollutants in aqueous environments. This is the rate of chemical decomposition in the aquatic environment induced by light or other radiant energy expressed as a DT50. Other information regarding, for example, pH sensitivity is also given in accompanying notes.</td></tr>
<tr><td>Aqueous hydrolysis DT50 (days) at 20^{o}C and pH 7:</td><td>This is the rate of chemical decomposition induced by water at pH 7 expressed as a DT50. Other information regarding, for example, pH sensitivity is also given in accompanying notes.</td></tr>
<tr><td>Water sediment study data: Water-sediment & Water phase only DT50s:</td><td>This is the rate of chemical decomposition in water-sediment systems expressed as a DT50. Data is given for the system as a whole and for the water phase only.</td></tr>
<tr><td>GUS leaching potential index:
NOTE: THIS IS AN INDICATOR & NOT A RISK ASSESSMENT</td><td>The GUS index (Groundwater Ubiquity Score) is a very simple indicator of a chemical potential for leaching into groundwater. It is based on the environmental fate properties of the chemical and takes no account of environmental conditions. It is not a substitute for modelling and risk assessment studies.
Calculated from the soil degradation rate (DT50) and the Organic-carbon sorption constant (koc) where:
GUS = log(DT50) x (4 - log (koc))
If GUS > 2.8 = likely to leach
If GUS < 1.8 = unlikely to leach
If GUS 1.8 - 2.8 = leaching potential is marginal
(Reference: Gustafson, D.I. (1989) Groundwater Ubiquity Score: A Simple Method for Assessing Pesticide Leachability Environmental Toxicology and Chemistry, 8, pp339-357).</td></tr>
<tr><td>SCI-Grow groundwater index:
NOTE: THIS IS AN INDICATOR & NOT A RISK ASSESSMENT</td><td>This is an indicator, used by the USEPA, to crudely estimate chemical (mainly pesticide) concentrations in vulnerable groundwater. It is based on environmental fate properties of the chemical, the application rate and existing data from small-scale monitoring studies. It is not a substitute for modelling and risk assessment studies.
(Ref: www.epa.gov/oppefed1/models/water/scigrow_description.htm)
Calculated from the soil degradation rate (DT50) and the Organic-carbon sorption constant (koc) where:
Step 1:
<table>
<tr><td>D = log(Koc + 5.0)</td><td></td><td></td></tr>
<tr><td>if DT50 < 6.0 then</td><td>C = log(DT50/6.0)</td><td>R = C * D</td></tr>
<tr><td>if DT50 6.0 - 1500 then</td><td>C = log(DT50 - 5.0)</td><td>R = C * (4-D)</td></tr>
<tr><td>if DT50 > 1500 then</td><td>C = log(1500) = 3.176</td><td>R = C * (4.-D)</td></tr>
</table></td></tr>
</table>

Parameter	Explanation		
	Step 2:		
	If Koc = 9995 then	F = -2.241 + 0.610 * R	Normalised concentration = 10^F
	If Koc > 9995 then	Normalised concentration = 0.006	