2.3. General physicochemical 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^{-1})	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^{-1})	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.
Fat solubility of residues	Fat-soluble pesticides are those that can be stored in the liver or in fatty tissues. Consequently, they may bioaccumulate and can be environmentally persistent. As a guide the value of Log P can be used. Where log P is greater than 3 the pesticide residue is likely to be soluble in fat but there are exceptions to this rule and so assessment using metabolism and farm animal feeding studies provides the most accurate guide. This information can be important for oil extraction processes as fat solubility will influence the concentration of a pesticide in the processed products.
Density	Parameter given depends on the physical state (solid or liquid) of the chemical (g ml^{-1}).
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 20°C. It is a measure of the tendency of a material to vaporise. The higher the vapour

	pressure the greater the potential. The short-range air transport exposure assessment scheme uses a vapour pressure trigger to identify substances of potential concern. The trigger is 10^{-2} mPa (at 20°C) if a substance is applied to plants and 10^{-1} mPa (at 20°C) if the substance is applied to soil. Substances that exceed these triggers, ideally require drift mitigation.
Henry's law constant Dimensional	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.m^3/mol.
Volatilisation as max % of applied dose lost (from plant surface & from soil surface)	The percentage of the applied dose lost from the plant and soil surface due to volatilisation at 20°C in the stated timeframe, which is normally 24 hrs. The trigger for concern is >= 20%[1]. For pesticides with volatilisation rates below 20% volatilisation is not considered as critical.
Max UV-Vis absorption (L mol^{-1} cm^{-1})	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.
Surface tension (mN m^{-1})	The tendency of the surface of to resist an external force.
Refractive index (VSDB only)	This is an optical term and is a dimensionless number that describes how light, or any other radiation, propagates through that medium.
Environmental release (VSDB only)	Main mechanisms of entry into the environment.
Degradation	
General biodegradability (PPDB only)	Short text giving comment on the general biodegradability of the pesticide in the environment.
Soil degradation DT50 Typical/Laboratory/Field - days	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. 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.*

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[1] 1 BBA - Biological Federal Institute for Agriculture and Forestry. (1990). Study of the Volatilisation Behaviour and Fate of Plant Protection Products in the Air - Guidelines for the Official Testing of Plant Protection Products, Part IV, 6-1, Braunschweig. [BBA - Biologische Bundesanstalt fur Land- und Forstwirtschaft (Juli 1990) Priifung des Verfluchtigungsverhaltens und des Verbleibs von Pflanzenschutzmitteln in der Luft. Richtlinien fur die amtliche Prufung von Pflanzenschutzmitteln, Teil IV, 6-1, Braunschweig.]

Manure DT_{50} - days (VSDB only)	The time required for the chemical concentration to decline to 50% in livestock manures.
Dissipation rate RL50 on plant matrix - days (PPDB/BPDB only)	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.).
Dissipation rate RL50 on and in plant matrix - days (PPDB/BPDB only)	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.).
Note: *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.*	
Aqueous photolysis DT50 (days at 20^{o}C pH 7)	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.
Aqueous hydrolysis DT50 (days at 20^{o}C and pH 7)	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.
Water sediment study data - Water-sediment & Water phase only DT50s	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.
Soil sorption K_{oc} / K_{foc}	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 (K_{oc}) and non-linear (K_{foc}) parameters are given. Three summary parameters are given for K_{foc} and two for K_{oc}.
Note: (i) *More detailed data where K_{oc}/K_{foc} 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.*	
GUS leaching potential index **NOTE: THIS IS AN INDICATOR & NOT A RISK ASSESSMENT**	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).

<table>
<tr><td rowspan="9">SCI-Grow groundwater index
NOTE: THIS IS AN INDICATOR & NOT A RISK ASSESSMENT</td><td colspan="4">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 (DT_{50}) and the Organic-carbon sorption constant (K_{foc} or K_{oc}) where:
Step 1:</td></tr>
<tr><td colspan="4">$CO = \log_{10}(K_{foc} + 5.0)$ OR $C = \log_{10}(K_{oc} + 5.0)$</td></tr>
<tr><td>if $DT_{50} < 6.0$ then</td><td colspan="2">$DT = \log_{10}(DT_{50}/6.0)$</td><td>RILP = DT * CO</td></tr>
<tr><td>if DT_{50} 6.0 - 1500 then</td><td colspan="2">$DT = \log_{10}(DT_{50} - 5.0)$</td><td rowspan="2">RILP = DT * (4 - CO)</td></tr>
<tr><td>if $DT_{50} > 1500$ then</td><td colspan="2">$DT = \log_{10}(1500) = 3.17609$</td></tr>
<tr><td colspan="4">**Step 2:**</td></tr>
<tr><td colspan="2">If K_{foc} or Koc <= 9995 then</td><td colspan="2">$SCI\text{-}GROW = 0.892 * 10^{(-2.241 + (0.61 * RILP))}$</td></tr>
<tr><td colspan="2">If K_{foc} or K_{oc} > 9995 then</td><td colspan="2">$SCI\text{-}GROW = 0.892 * 0.006$</td></tr>
<tr><td colspan="4">**Note:** US developed SCI-GROW assumes an application rate of 1lb a.i/acre, therefore the 0.892 is included to convert it to kg a.i./ha.</td></tr>
<tr><td>Potential for particle bound transport index</td><td colspan="4">An indicator of the general potential for particle bound transport index.</td></tr>
<tr><td>Potential for loss via drain flow</td><td colspan="4">An indicator of the general potential for the loss of a substance via drain flow (derived from k_{oc}/k_{foc})</td></tr>
<tr><td>Photochemical oxidative DT_{50} (hrs) as indicator of long-range air transport risk</td><td colspan="4">Photo-oxidative processes (indirect photolysis) and light-induced reactions (direct photolysis) are the main transformation pathways for pesticides in the atmosphere. Long-range air transport of pesticides will occur when compounds have a significant lifetime in air[2]. Reactions with hydroxy (OH^-) radicals are considered to be the major degradation process for most air pollutants, including pesticides due to the reaction with double bonds, the H abstractive power of hydroxyl and its high electrophilicity[3]. Due to issues of practicality, cost and unreliability the rate of degradation in air due to photochemical oxidation for pesticide risk assessments tends to be calculated using the method proposed by[3]. The EU FOCUS working group recommend a trigger of a DT50 in air of 2 days (48 hrs) to identify substances of potential concern for long-range transport[4]. In order to standardise the input parameters for the Atkinson calculation the Focus working group propose that a 12-hr day is used with a hydroxyl radical concentration of 1.5 x 106 OH radicals/cm^3.</td></tr>
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[2] Atkinson, R., Guicherit, R., Hites, R.A., Palm, W.-U., Seiber, J.N. and de Voogt, P. (1999). Transformation of pesticides in the atmosphere: a state of the art. Water, Air and Soil Pollut., 115: 219-243.

[3] Atkinson, R., Darnall, K.R., Lloyd, A.C., Winer, A.M. and Pitts, J.N. Jr. (1979). Kinetics and mechanisms of the reaction of the hydroxyl radical with organic compounds in the gas phase. *Advances in Photochemistry*, 11: 375-488.

[4] FOCUS. (2008). *Pesticides in Air: Considerations for Exposure Assessment.* Report prepared by the FOCUS Working Group on Pesticides in Air. European Commission report. SANCO/10553/2006 Rev 2 June 2008.

Bio-concentration factor	The concentration of the chemical in tissue per concentration of chemical in water. This describes the accumulation of pollutants through chemical partitioning from the aqueous phase into an organic phase, such as the gill of a fish.