The University of Hertfordshire Agricultural Substances Database Background and Support Information

The present document aims at providing information regarding the PPDB, BPDB and the VSDB, their management and data acquisition. It seeks to answer common questions regarding these matters. Information on the Terms and Conditions of use for each database can be found in a document that is available on the database website as a PDF download.

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What are the UH Agricultural Substances Databases?

The University of Hertfordshire's (UH) Agriculture & Environment Research Unit (AERU) have developed three databases relating to chemical (natural and synthetic) substances used in agriculture: pesticides, biopesticides and veterinary substances.

The Pesticide Properties Database (PPDB) is a comprehensive relational database of pesticide physicochemical, toxicological, ecotoxicological, human health and other related data. It contains data relating to synthetic pesticides and their metabolites. It has evolved from a database that originally accompanied the EMA (Environmental Management for Agriculture) software (also developed by AERU) and has been systematically developed further and expanded with funding from other research projects and earned income.

The BioPesticides Database (BPDB) is similar to the PPDB but contains data for biological pesticides – those that have been derived from natural substances such as plants. This was developed when the PPDB became very large and its was advantageous from a management point of view to separate certain records out, especially as the BPDB contains data not relevant to the PPDB such as taxonomic classifications and substance source.

The veterinary Substance Database (VSDB) contains data relating to substances used to manage the health and welfare of animals (mostly farmed livestock). It evolved in the same way as the BPDB as it also contains data not relevant to the PPDB or the BPDB such as pharmacological data relating to the drug or treatment activity..

How do the databases work?

The data is collated and stored in an MS Access database. A Microsoft Visual Basic data management application has been developed to manage the data adhering to strict formatting and quality control protocols and to keep track of versions, literature references and record cross-referencing. Another Visual Basic application is used to filter the data, handle the translations and generate the thousands of HTML pages for the PPDB website.

Explanation of the Terms and Parameters Used

(1) General chemical status information – descriptors and registration

Parameter	Explanation
Alias's/synonyms:	Other names by which the substance is known. These are enabled in the various database search facilities.
Description:	General description of the major uses of the substance.
Introduction:	Year (and country where known) of introduction, registration or discovery.
EU approval:	Provides an indication of where the active substance has been authorised for agricultural use within the EU. Please check with the relevant national authority before relying on this data.
EC Directive status (PPDB/BPDB only)	Status of the chemical in the EU peer review process EC directive 1107/2009 (repealing 91/414) of pesticide/biopesticide active substances.
Also registered in:	Other countries where we believe the substance is used. Please check

	with the relevant national authority before relying on this data.
Pesticide or veterinary substance type:	The specific type of substance described according to the type of pest or disease they control e.g. Insecticide, Herbicide, Fungicide, Acaricide, Antiparasitic, Anthelmintic etc.
Chemical group:	Chemical classification group based on the chemical structure.
Taxonomic classification (BPDB only)	A description of the natural substance according to its scientific taxonomy e.g. Kingdom, class, order, family, genus and species.
Chiral molecule:	A chiral molecule is a type of molecule that has a non-superimposable mirror image.
Mode of action:	The mechanism by which the substance performs its main function.
Target pest and host (BPDB only):	The pest or disease the substance is used to control and the crops it is used on.
Species treated (VSDB only)	Examples of the species which the drug may be used for.
Therapeutic class (VSDB only)	Description of the drugs activity according to its therapeutic activity.
Molecular target (VSD only)	This is the key molecule involved in a particular metabolic or signaling pathway that is specific to the disease condition or pathology or to the infectivity or survival of a microbial pathogen.
Metabolite type:	General description of the host process that creates the metabolite e.g. soil, water, animal, plant, groundwater.
Other constituent type:	General description of the purpose of the constituent in the formulation i.e. solvent, wetter, carrier etc.
CAS RN:	Chemical Abstracts Service Registry Number - a unique identify for the chemical.
EC number:	The unique reference number for the chemical in the European Chemical Substances Information System (EINECS) or European List of Notified Chemicals (ELINCS).
CIPAC number:	The CIPAC code number system is a simple approach for an unambiguous coding of chemicals. CIPAC, FAO, WHO and the EU are the main users of this system.
US EPA chemical code (PPDB/BPDB only):	The U.S. Environmental Protection Agency (U.S. EPA) assigns a unique reference number to individual pesticide active ingredients to assist in their identification. This code is sometimes referred to as the Shaugnessy Number.
ATCVet code (VSDB only)	A classification system is used to classify the drug/treatment according to its therapeutic action. This is similar to that used for human medicine.
Chemical formula:	This is a concise way of expressing information about the atoms that constitute the chemical.
SMILES:	The **S**implified **M**olecular **I**nput **L**ine **E**ntry **S**pecification (SMILES) is a specification for describing the structure of chemical molecules using short ASCII strings. SMILES strings can be imported by most molecule editors for conversion back into drawings or models of the molecules. Either the standard SMILES or the Canonical SMILES are given
InChl Identifier:	IUPAC **In**ternational **Ch**emical **I**dentifier. This is a textual identification for chemical substances, that provides a standard, readable way of encoding molecular information and to facilitate the search for such information in databases and on the web.
Structure diagram available	Either Yes or No. If Yes is stated this will be a link to a separate window displaying the structure diagram.

Molecular mass:	The relative molecular mass (molecular weight) of a chemical is the mass of a molecule of the chemical relative to the mass of a carbon atom taken as exactly 12.
Chemical name:	Name of the chemical according to the nomenclature rules of IUPAC or CAS. Where this is not available or does not apply a generic name is given.
Other status information:	This will display information relating to the status of the substance with respect to other legislation, international conventions and information regarding phase out. Including: **PIC Annex 1 chemicals:** The Rotterdam Convention on Prior Informed Consent (PIC). The Convention covers pesticides and industrial chemicals that have been banned or severely restricted for health or environmental reasons by parties and which have been notified for inclusion in the PIC procedure by those parties. One notification from each of two specified regions triggers consideration of addition of a chemical to Annex III of the Convention. Severely hazardous product formulations that present a hazard under conditions of use in developing may also be nominated for inclusion in Annex III. **POP chemicals:** The Stockholm Convention on Persistent Organic Pollutants (POP). POPs are exceedingly toxic chemicals that are extremely persistent in the environment, travel long distances on wind and water currents, and concentrate up the food chain to accumulate in our bodies. They also have serious health implications and can cause cancer, neurological and learning disabilities, and subtle changes to human reproductive and immune systems. The Stockholm Convention bans or severely restricts the most hazardous POPs, and establishes an international, science-based process for adding other POPs to the treaty. Those listed in this database also include chemicals that are new POP candidates proposed by other organisations including the WWF. **VOC chemicals: Volatile organic compounds** (**VOCs**) are organic chemical compounds that have high enough vapour pressures under normal conditions to significantly vaporise and enter the atmosphere. The term VOC may have special legal meanings in some countries. **LRTAP Chemicals:** The Convention on Long-range Transboundary Air Pollution (LRTAP): The aim of the Convention is that Parties seek to limit and, as far as possible, gradually reduce and prevent air pollution including long-range transboundary air pollution. Chemicals considered to be the most serious problem are assigned to Annex 1. **PAN Dirty Dozen / PAN Bad Actor:** The Pesticide Action Network (PAN) have identified these chemicals as being particularly harmful. **OSPAR:** OSPAR Convention for the Protection of the Marine Environment: pfa - priority substances for action, soc - substances of concern. **WFD:** Water Framework Directive 2000/60/EC: phs - priority hazardous substance, pps - possible priority substance, other - other substance of concern. **Groundwater contaminant:** substance is known to have polluted groundwaters and is a substance of concern.
Resistance code (PPDB/BPDB only:	This is the HRAC, IRAC or FRAC code that denotes their resistance classification and can be used in resistance management programmes.
Physical state:	Provides an indication of the physical state of the material – solid,

	liquid or gas and its general appearance. This normally applies to the active substance in its pure state unless stated otherwise.

(2) General product and branding information

Parameter	Explanation
Example manufacturers &/or suppliers	Examples of companies who have manufactured, supplied or used the substance in their products.
Example products:	Non-exhaustive list of examples of products that include the substance.
Associated substances:	Non-exhaustive list of other substances associated with the substance. These may include other pesticides, solvents, inerts and impurities or concern. Links cross-referencing to the associated substances are supplied.
UK LERAP status (PPDB only):	Classification of the substance (where applicable) regarding its UK LERAP (Local Environmental Risk Assessment for Pesticides) status and the need for 'No spray' zones adjacent to surface water bodies.
Formulation & application details:	This provides brief information on the main types of formulations and aspects relating to their application.

(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.
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.
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.
Aqueous photolysis DT50 (days) at 20°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°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.

<table>
<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>
<tr><td colspan="3">Step 2:</td></tr>
<tr><td>If Koc = 9995 then</td><td>F = -2.241 + 0.610 * R</td><td>Normalised concentration = 10^F</td></tr>
<tr><td>If Koc > 9995 then</td><td colspan="2">Normalised concentration = 0.006</td></tr>
</table></td></tr>
<tr><td></td><td>Step 3:
Total chemical use = application rate (kg/ha) * number of applications
Estimated concentration in groundwater = Normalised concentration * total chemical use
(Reference: www.oecd.org/dataoecd/6/17/2752913.pdf)</td></tr>
<tr><td>Potential for particle bound transport index:
NOTE: THIS IS AN INDICATOR & NOT A RISK ASSESSMENT</td><td>This is a simple indicator of a chemicals (usually pesticides) run-off potential. It classifies chemicals into three broad risk categories based on environmental fate properties. It takes no account of environmental or landscape conditions. It is not a substitute for modelling and risk assessment studies.</td></tr>
<tr><td>Koc (Kfoc) - organic-carbon sorption constant: (mL/g)</td><td>Chemicals vary in how well they are adsorbed to soil particles. Koc / Kfoc measures the affinity for chemicals to sorb to organic carbon. The higher the value, the stronger the tendency to attach to and move with soil. Koc / Kfoc values greater than 1,000 indicate strong adsorption to soil. Chemicals with lower Koc / Kfoc values (less than 500) tend to move more with water than adsorbed to sediment.</td></tr>
</table>

	Some chemicals are strongly bound to other soil components such as clay surfaces. For some chemicals Koc/ Kfoc will be very sensitive to pH.
Freundlich coeffts (Kf and $^{1}/_{n}$):	A 'soil absorption coefficient' study is to predict the mobility of a chemical in the environment. If carried out over a range of chemical concentrations the result can be fitted to an equation called the 'Freundlich isotherm', that is used to describing adsorption. This equation is $Q=kC^{1}/_{n}$, where Q is the amount of the sorbed chemical in equilibrium, C is the concentration of the chemical in solution, *K* and *n* are empirical constants, *Kf* is called the sorption coefficient. An *n* value of 1 denotes a linear sorption process.

(4) Metabolite/Parent information

Parameter	Explanation
Metabolites:	A chemical degradation product - a chemical product formed upon the breakdown of a chemical. Any significant or important metabolites are shown (predominately those formed in the soil) together with links to their profile pages. This list is not exhaustive. Links cross-referencing to the metabolites are supplied.
Parent:	The parent substance that has degraded to produce the metabolite.
Formation media:	The host process that creates the metabolite e.g. soil, water, animal, plant, groundwater.
Estimated Maximum Occurrence (PPDB/BPDB only:	The maximum amount of the named metabolite identified (via soil degradation studies) in the formation media expressed as a fraction of the chemical applied.
91/414 Relevancy	Within Directive 91/414 a metabolite is considered to be 'relevant': - if there is reason to believe that it has comparable intrinisic properties to the parent chemical in terms of its biological target activity, or if it - has toxicological properties that are considered severe, or - poses a higher or comparable risk to organisms than the parent substance. Therefore 'relevant' metabolites may need to so be taken into account within any risk assessment process. Please note that some regulatory dossiers (pesticides) pre-date the introduction of 'relevant metabolites' and, instead, declared metabolites as 'Major' if their estimated maximum occurrence fraction >10%.
Other metabolites	Basic information may also be given for other metabolites where data is limited.

(5) Ecotoxicology

Parameter	Explanation
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.
Bioaccumulation potential:	The potential for an organism to absorbs the chemical at a rate greater than that at which the substance is lost from the body.

Fauna and flora ecotoxicological endpoint data:	Data used to measure the adverse effects on living organisms that chemicals can have when released into the natural environment. See **Endpoint Glossary and Key Species data** below.
Mesocosm study data:	Mesocosm studies are a useful tool for higher-tier aquatic risk assessment. They are widely used in the regulatory assessment processes to evaluate the effects of chemical pollutants on aquatic communities at the ecosystem level.

(6) Human health

Parameter	Explanation
Toxicity endpoints for mammals:	Oral, dermal and inhalation values provided.
WHO classification:	Toxicity hazard class given by the World Health Organisation (WHO). Class Ia: extremely hazardous Class Ib: highly hazardous Class II: moderately hazardous Class III: slightly hazardous O: Obsolete substance NL: Not listed The system is based on the LD50 endpoint for rats. An ingested solid with a LD50 5mg or less/kg bodyweight is Class Ia, at 5-50 mg/kg Class Ib, at 50-500 mg/kg Class II, and at more than 500 mg/kg Class III. Values may differ for liquid oral agents and dermal agents.
US EPA acute toxicity class (formulation, pesticides), PPDB/BPDB only	Toxicity hazard class of the formulation as given by the EPA. Class 1: Highly toxic Class II: Moderately toxic Class III: Slightly toxic Class IV: Not acutely toxic
US EPA classification for products (PPDB/BPDB only):	This is the hazard class assigned to chemical (usually pesticides) products containing the active substance. Generally, Class I substances will kill an adult person at a dose of less than 5g, Class II at 5-30g, and Class III >30g.
CLP classification	The 'CLP' Regulation (EC) No 1272/2008 on the classification, labelling and packaging of substances and mixtures, or simply 'CLP', introduces the United Nations globally harmonised system (UN GHS) for classification and labelling of chemicals into Europe. For further information on this please see other documents available on the PPDB website under Support Information/Other Information.
EC risk classification / safety classification:	EC Directive 67/548/EEC provides a harmonised basis for the classification (risk) and handling (safety) of dangerous substances. These listed here are those for the active substance. More details of what the specific codes means can be found on the PPDB website, in the downloads section.
Acceptable Daily Intake – ADI mg kg^{-1} bw day^{-1}:	The amount of chemical that can be consumed each day without causing harm - as far as evidence suggests.
Acute Reference Dose – ARfd mg kg^{-1} bw day^{-1}::	The amount of chemical that can be ingested over a short period of time, usually during one meal or one day, without appreciable health risk to the consumer - as far as evidence suggests.

Acceptable Operator Exposure Level mg kg^{-1}bw day^{-1}: - AOEL:	This is a health-based limit that is established on the basis of the full toxicological assessment required for regulatory purposes. The risk for operators can be quantified by comparing this value with exposure level during application.
Dermal penetration studies %	Mean value of known studies reported. Default value in the absence of further evidence is normally taken as 10%.
Dangerous substances Directive:	This Directive concerns pollution caused by certain dangerous substances discharged into the aquatic environment and aims to regulate potential aquatic pollution. The Directive covered discharges to inland surface waters, territorial waters, inland coastal waters and groundwater. The protection of groundwater is now regulated under a separate Council Directive. Directive 76/464 introduced the concept of list I and list II chemicals. Where the chemical concerned appears on these lists it is given here.
Exposure limits:	Exposure of employees, operators and other workers to hazardous substances should be prevented and in some cases national or EC regulations impose limits. Where identified these are quoted and may include Maximum Exposure Limits (MEL), Occupational Exposure Standards (OES) and Short Term Exposure Limits (STEL). List is not exhaustive but given for guidance only.
Exposure routes public and occupational:	Where identified risks to the public (e.g. bystanders and consumers) and operators/workers are identified. This list is not exhaustive but given for guidance only.
EU MRLs mg kg^{-1}	MRLs are defined as the maximum concentration of chemical residue likely to occur in or on food, drink and feeding stuffs after the use of chemicals according to Good Practice (GP). GP is defined as the substance being applied in accordance with current regulations, product label recommendations and in keeping with local environmental and other conditions. The values listed here are for guidance only and are often those proposed within regulatory documents. More precise information on pesticides and biopesticides can be found in the EU Database.
Drinking water MAC:	The Maximum Acceptable Concentration of the chemical in drinking water.
General health issues:	Summary of main issues relating to human health. This list is not exhaustive and for guidance only.
Specific health issues:	Summary of the main human health concerns across a number of issues. Note this is somewhat subjective as literature is not universally uniform in the way issues are addressed. We have used a 'weight-of-the-evidence' approach erring on the side of caution.
Handling issues:	General description of any hazards that should be addressed when handling the substances.

(7) Translations

Language translations for the common name by which the substance is now is provided (where known) in English, French, German, Danish, Italian, Spanish, Greek, Slovenian, Polish, Swedish, Hungarian and Dutch within each substance record. The entire PPDB database is also currently available in a range of European languages. However, please note the language

translation of these databases is no longer supported and these databases are currently being phased out.

The Primary Data Sources Used to Populate the databases

We use mainly public domain sources (mainly that of regulatory bodies), peer reviewed literature and private databases with copyright/IPR permission where required.

Note: This list is non-exclusive and just provides an example of the sources utilised

A	EU Regulatory & Evaluation Data as published by EC, EFSA (DAR & Conclusion dossiers), EMA / EU Annex III PIC DGD / EU MRL Database (See http://ec.europa.eu/sanco_pesticides/public/index.cfm)
AA	IOBC Database on classification of side effects to beneficial organisms, 2005
AB	SELECTV Database (See http://ipmnet.org/phosure/database/selctv/selctv.htm)
AC	EC Joint Research Centre ESIS European Chemical Substance Information Systems including EINECS (See http://ecb.jrc.ec.europa.eu/esis/)
AE	Joint Assessment of Commodity Chemicals ECETOC (See http://www.ecetoc.org)
AF	European Food Safety Agency (EFSA)
B	UK CRD and ACP Evaluation Documents / and other DEFRA (UK) documents (See http://www.pesticides.gov.uk/publications.asp?id=202)
C	AGRITIX (See http://www.dive.afssa.fr/agritox/index.php)
CA	Medical and toxicological databases and information systems e.g. TOXNET (See http://toxnet.nlm.nih.gov/cgi-bin/sis/htmlgen?HSDB)
D	Agricultural Research Information System (ARIS) Database
DW	Don Wauchope personal database for Pka data: Wauchope, R. D. and Edwards, J. Dissociation constants for pesticide active ingredients: a database and comparison with predicted values. MS in preparation
E	Manufacturers Safety Data Sheets
F	U.S. EPA ECOTOX Database (see http://cfpub.epa.gov/ecotox/) / U.S. EPA Pesticide Fate Database (See http://cfpub.epa.gov/pfate/home.cfm) / Miscellaneous WHO documents.
FAO	Miscellaneous FAO publications
G	Extension Toxicology network Database EXTOXNET (See http://extoxnet.orst.edu/ghindex.html)
H	The US ARS Pesticide Properties Database (See http://www.ars.usda.gov/Services/docs.htm?docid=14199)
J	Pesticide Action Network Database (See http://www.pesticideinfo.org/)
K	Research Datasets (e.g. Pandora, Demetra (see http://www.demetra-tox.net/))
L	Pesticide manuals and hard copy reference books / other sources
M	GLEAMS Model database (Groundwater Loading Effects of Agricultural Management Systems). (See http://www.cpes.peachnet.edu/sewrl/Gleams/gleams_y2k_update.htm)
N	Various Trusts, NGOs & Charities Data
P	Other Governments and Regulators
O	Miscellaneous Data From On-line Sources
R	Peer Reviewed Scientific Publications
S	Expert Judgement
T	UN EPFA Database
US	US Dept of Agriculture National Resources Conservation Service - various datasheets, databases and online sources

V	ChemID Online Databases (See http://chem.sis.nlm.nih.gov/chemidplus/) / IPCS INCHEM (See http://www.inchem.org/)
W	French database provided by ARVALIS-Institut du Végétal
X	WINPST Database (See http://www.ipm.ucdavis.edu/TOX/winpstdoc.html)
Y	Germany's Federal Environment Agency (UBA) (See http://www.umweltbundesamt.de/index-e.htm)
Z	Kingtai Chemials Website (See http://www.kingtaichem.com/)

Data Interpretation

(1) Environmental fate

Parameter	Source	Thresholds
Solubility in water (mg l^{-1}):	Arbitrary system in common use	<= 50 = Low 50 - 500 = Moderate > 500 = High
Octanol-water Partition Coefft (Log P):	Used by the US EPA. Widely used rule of thumb.	< 2.7 = Low bioaccumulation 2.7 – 3 = Moderate > 3.0 = High
Soil degradation (days):	See note 1.	< 30 = Non-persistent 30 - 100 = Moderately persistent 100 - 365 = Persistent > 365 = Very persistent
Aqueous photolysis DT50 (days) at pH 7:	See note 5.	< 1 = Fast 1 - 14 = Moderately fast 14 - 30 = Slow > 30 = Stable
Aqueous hydrolysis DT50 (days) at 20°C and pH 7:	See note 5.	< 30 = Non-persistent 30 - 100 = Moderately persistent 100 - 365 = Persistent > 365 = Very persistent
Water-sediment degradation (days):	Same thresholds as soil degradation utilised. See note 1.	< 30 = Fast 30 - 100 = Moderately fast 100 - 365 = Slow > 365 = Stable
Water phase only degradation (days):	See note 5.	< 1 = Fast 1 - 14 = Moderately fast 14 - 30 = Slow > 30 = Stable
GUS Index:	Gustafson, DI (1989) Groundwater Ubiquity Score: a simple method for assessing chemical leachability. Environ. Toxicol. Chem 8, 339-357.	> 2.8 = High leachability 2.8 - 1.8 = Transition state < 1.8 = Low leachability
Koc/ Kfoc (ml g^{-1}):	PSD Pesticide Data Requirement Handbook (2005). SSLRC Mobility Classification System. Also	< 15 = Very mobile 15 - 75 = Mobile 75 - 500 = Moderately mobile 500 - 4000 = Slightly mobile

	See note 5.	> 4000 = Non-mobile
Vapour pressure at 25°C (mPa):	Kerle EA, Jenkins JJ & Vogue PA (1996) Understanding pesticide persistence and mobility for groundwater and surface water protection. Oregon State University. EM 8561.	< 1 x 10^{-6} = Non-volatile 1 X 10^{-4} - 1 x 10^{-6} = Intermediate state > 1 X 10^{-4} = Volatile
Henry's Law Constant at 20°C (Dimensionless - K_H):	See note 2.	> 2.5 x 10^{-5} = Volatile 2.5 x 10^{-7} - 2.5 x 10^{-5} = Moderate volatility < 2.5 x 10^{-7} = Non volatile
Henry's Law Constant (Pa m^3 mol^{-1}):	Rule of thumb in wide, general use.	> 100 = Volatile 0.1 - 100 = Moderately volatile < 0.1 = Non-volatile
Particle Bound Transport Indicator:	Goss & Wauchope (1990). See note 3.	
SCIGROW Indicator:	See note 10.	
Freundlich equation:	See note 11.	

(2) Ecotoxicology

Parameter	Source	Thresholds
Bio-concentration factor:	General rule of thumb and that used by the US EPA.	< 100 = Low potential 5000 – 100 = Threshold for concern > 5000 – High potential
Bioaccumulation potential:	See note 7.	See note 7.
Mammals - Acute oral LD50 (mg kg^{-1}):	See note 5.	> 2000 = Low 100-2000 = Moderate < 100 = High
Mammals - Short term dietary NOEL (mg kg^{-1}):	See note See note 5.	> 2000 = Low 100-2000 = Moderate < 100 = High
Birds - Acute LD50 (mg kg^{-1}):	Consistent with US EPA Guidelines. See note 5.	> 2000 = Low 100 - 2000 = Moderate < 100 = High
Fish - Acute 96 hour LC50 (mg l^{-1}):	See note 5.	> 100 = Low 0.1 - 100 = Moderate < 0.1 = High
Fish - Chronic 21 day NOEC (mg l^{-1}):	See note 5.	> 10 = Low 0.01 - 10 = Moderate < 0.01 = High
Aquatic invertebrates - Acute 48 hour EC50 (mg l^{-1}):	See note 5.	> 100 = Low 0.1 - 100 = Moderate < 0.1 = High
Aquatic invertebrates - Chronic 21 day NOEC (mg l^{-1}):	See note 5.	> 10 = Low 0.01 - 10 = Moderate < 0.01 = High
Aquatic crustaceans - Acute 96 hour LC50 (mg l^{-1}):	See note 5.	> 100 = Low 0.1 - 100 = Moderate < 0.1 = High

Sediment dwelling organisms - Acute 96 hour LC50 (mg l^{-1}):		See note 5.	> 100 = Low 0.1 - 100 = Moderate < 0.1 = High
Sediment dwelling organisms - Chronic 28 day NOEC, static, water (mg l^{-1}):		See note 5.	> 10 = Low 0.01 - 10 = Moderate < 0.01 = High
Sediment dwelling organisms - Chronic 28 day NOEC, sediment (mg kg^{-1}):		See note 5.	> 100 = Low 0.1 - 100 = Moderate < 0.1 = High
Aquatic plants - Acute 7 day EC50, biomass (mg l^{-1}):		See note 6.	> 10 = Low 0.01 - 10 = Moderate < 0.01 = High
Algae - Acute 72 hour EC50, growth (mg l^{-1}):		See note 6.	> 10 = Low 0.01 - 10 = Moderate < 0.01 = High
Algae - Chronic 96 hour NOEC, growth (mg l^{-1}):		See note 6.	> 1 = Low 0.001 - 1 = Moderate < 0.001 = High
Honeybees - Acute 48 hour LD50 (µg bee^{-1}):		See note 5.	> 100 = Low 1 - 100 = Moderate < 1 = High
Earthworms - Acute 14 day LC50 (mg kg^{-1}):		See note 12.	> 1000 = Low 10 - 1000 = Moderate < 10 - High
Earthworms - Chronic 14 day NOEC, reproduction (mg kg^{-1}):		See note 12.	> 100 = Low 0.1 - 100 = Moderate < 0.1 = High
Other soil macro-organisms:	LR50 / EC50 / NOEC / % Effect:	See note 13.	No interpretation
Other arthropods:	LR50 data:	See note 8.	< 50 = Harmful at 1kg ha^{-1} 50-500 = Moderately harmful at 1kg ha^{-1} > 500 = Harmless at 1kg ha^{-1}
	% Effect data:	See note 9.	< 30 = Harmless 30 - 79 = Moderately harmful > 79 = Harmful
Soil micro-organisms:		Nitrogen / carbon mineralisation.	<= 25% change is considered insignificant.

(3) Human health

Parameter	Source	Thresholds
Who Toxicity class:	WHO Guidelines 2004. Based on rat LD50 & physical state of the pesticide. See note 4.	See note 2.
EPA acute toxicity class (formulation):	Standard text book thresholds. These apply to the formulated product.	I - Highly toxic II - Moderately toxic III - Slightly toxic IV - Not acutely toxic In some instances there is slight variation in product

		classification. In these instances multiple listings are given, unless there is no consensus across brands in which case the text reads 'No consensus across products'.
EC Risk classification:	Risk Information contained with in Annex II and III of Directive 67/548/EEC on Classification and Labelling of Dangerous Substances.	
EC Safety classification:	Safety Information contained with in Annex IV of Directive 67/548/EEC on Classification and Labelling of Dangerous Substances.	
ADI (mg kg^{-1} bw):	The acceptable daily intake is the amount of a substance that can be ingested every day of an individual's entire lifetime, in the practical certainty, on the basis of all known facts, that no harm will result. SF – refers to the safety factor applied.	
AOEL (mg kg^{-1}):	The acceptable operator exposure level is the maximum amount of active substance to which the operator may be exposed without any adverse health effects. SF – refers to the safety factor applied.	
Dangerous substances directive:	This Directive requires Member States to introduce measures to eliminate (List I) or to reduce (List II) pollution of the aquatic environment from certain listed substances identified in its Annexes.	
Exposure limits:	An exposure limit is the concentration of a chemical in the workplace air to which most people can be exposed without experiencing harmful effects.	
MRL's - maximum residue limits:	These limits can change and the data given here is usually that proposed by EFSA. Data may not be complete. See EU database for further information.	
Drinking water MAC:	Maximum Admissible Concentration of the chemical in drinking water. The MAC for a chemical is derived from its ADI. The EU Drinking Water Directive imposes a maximum admissible concentration (EU MAC) for any individual pesticide compound of 0.1 mg l^{-1}.	

Notes

1. Consistent with EU Guidance. (9188/VI/97 rev. 8.) and
    I. Kerle EA, Jenkins JJ & Vogue PA (1996), Understanding pesticide persistence and mobility for groundwater and surface water protection. Oregon State University. EM 8561.
    II. Rao PSC & Hornsby AG (2004) Behaviour of pesticides in Soils and water. University of Florida. See http://edis.ifas.ufl.edu/SS111.
    III. See also Note 3 below.

2. Several relevant references which include:
    I. Van der Werf , HMG (1996) Assessing the impact of pesticides on the environment. Agriculture, Ecosystems & Environment, 60, 81-96.

II. Jury WA, Spencer WF, & Farmer WJ (1984) Behaviour assessment model for trace organics in soil. III Application of screening model. J. Environ Qual. 13, 573-579.

III. Kerle EA, Jenkins JJ & Vogue PA (1996) Understanding pesticide persistence and mobility for groundwater and surface water protection. Oregon State University. EM 8561.

3. Table below has been extracted from:

I. Goss, D & Wauchope RD (1990) The SCR/ARS/CES Pesticide Properties Database. II using it with Soils data in a screening Procedure. In D.L. Weigmann Ed., Pesticides in the next decade: the challenge ahead, Virginia Resources Research Centre, Blacksburg, VA, USA pp471-493.

Potential for Particle-bound transport	**Criteria**
High	DT50 >= 40 days & Koc >= 1000 DT50 >= 40 days, Koc >= 500 & solubility = 0.5 mg/l
Low	DT50 <= 1 day DT50 <= 2 days & koc <= 500 DT50 <= 4 days, Koc <= 900 & solubility >= 0.5 mg/l DT50 <= 40 days, Koc <= 500 & solubility >= 0.5 mg/l DT50 <= 40 days, Koc <= 900 & solubility >= 2 mg/l
Medium	All other

4. Classification given below has been extracted from the WHO Guidelines document: The WHO recommended classification of pesticides by hazard & guidelines to classification. (2004). See http://www.who.int/publications/en/

Class Ia: extremely hazardous
Class Ib: highly hazardous
Class II: moderately hazardous
Class III: slightly hazardous
O: Obsolete
NL: Not listed

5. Thresholds used have been selected to be consistent with industry guidelines, were developed, and are consistent with regulatory thresholds used in both the UK and EU.

6. The EU (Uniform Principles) (Annex VI of Directive 91/414/EEC) guidelines have been adopted have set toxicity:exposure (TER) ratios for algae and aquatic plants at $^{1}/_{10}$th of those for fish and daphnids. The same ratio has been applied here.

7. Deleted

8. In EU pesticide regulatory risk assessments 'hazard quotients' are used to determine the need for additional studies to assess risk to beneficial arthropods. Hazard quotients (HQ) are determined by dividing the application rate of the active substance by the median lethal rate (LR50). HQ values less than 2.0 are considered to be low risk to beneficial arthropods and additional (higher tier) data is not required. Values greater than 2.0 trigger additional data requirements. The risk phrases quoted within this database are based on a standard application rate of 1 kg ha-1 and should be taken as **a comparative guideline only**. For a more accurate assessment divide the actual application rate of the active substance (in

grams) by the LR50 value quoted. Any value less than 2.0 can be considered a low risk. Values greater than 2.0 may require care and mitigation. Please note the thresholds for moderate and high risk are **arbitary values**.

9. Where two values are given (e.g. mortality / parsitism), base assessment on the highest absolute value (i.e. can be a positive or negative effect).

10. SCI-GROW is a screening model used by the US EPA to estimate pesticide concentrations in vulnerable groundwater. The model provides an exposure value that can be used to determine the potential risk to the environment and to human health from drinking water contaminated with the pesticide. The SCI-GROW estimate is based on environmental fate properties of the pesticide (aerobic soil degradation half-life and linear adsorption coefficient normalised for soil organic carbon content), the maximum application rate, and existing data from small-scale prospective ground-water monitoring studies at sites with sandy soils and shallow ground water.

    SCI-GROW estimates represent worse case estimates. For this reason, it is not appropriate to use SCI-GROW concentrations for national or regional exposure estimates. Nor is this indicator an alternative to a scientific risk assessment. Values given are based on a standard 1 kg ha^{-1} or 1 L ha^{-1} application rate and should be adjusted to the actual application rate used

    For more information see:
    http://www.epa.gov/oppefed1/models/water/scigrow_description.htm.

11. The distribution of a pesticide between the solution and absorbed phases can often be described by the "Freundlich equation", an equation that is used to describe a wide variety of adsorption data from every area of science. The equilibrium concentration and adsorbed pesticide amounts are determined experimentally. The Log_{10} of the quantity of adsorbed pesticide is plotted against the equilibrium concentrations. Often the relationship obtained is approximately linear and can be described by the Freundlich equation: $Q=KC^{1/n}$, where Q is the adsorbed amount of pesticide (µg kg^{-1}), C is the equilibrium concentration (µg l^{-1}), and kf and n are the experimental parameters unique to the isotherm. The parameter n is greater than 1, the larger it is the more non-linear the equation becomes.

12. The availability of the pesticide in the soil can depend on the amount of soil organic carbon (SOC). The toxicity endpoint value may therefore be corrected for the difference in SOC of the test soil and the reference soil. This means that the toxicity endpoint value is divided by the percentage organic matter in the standard test soil, and multiplied by the percentage organic matter in the reference soil. Uncorrected values are quoted herein unless otherwise stated e.g. '(corr)'.

13. Data is very limited and is presented in the literature in a variety of formats. Therefore neither a standard format nor interpretation can be provided.

Key Species and Endpoint Glossary

Parameter	Explanation
EC50:	The concentration of a chemical that can be expected to cause a defined non-lethal effect in 50 per cent of the tested population. In some cases other percentages may be displayed e.g. EC10 or EC15.
LD50:	Used in toxicology this is the median lethal dose (LD_{50}, abbreviation for 'Lethal Dose, 50%'), of a toxic substance and is the dose required to kill half the tested population. LD_{50} figures are frequently used as a general indicator of a substance's acute toxicity.
NOEL/NOEC:	Greatest concentration or level of a substance, found by observation or experiment, which causes no detectable effect.
NOEAEC:	'No Observed Ecologically Adverse Effect Concentration' - the highest concentration that causes no observed adverse effect on fauna or flora.

Species	Explanation
Given below are the first choice species for ecotoxicological endpoints. However, if these are not available data for other species may be given instead. This will be indicated in the accompanying notes. Where data for several species are available, data for the most sensitive is given.	
Mammals	Rat, Mice, Dog (Mainly used for the human health studies)
Birds	Mallard duck (*Anas platyrhynchos*) Bobwhite quail (*Colinus virginianus*)
Fish	Rainbow trout (*Oncorhynchus mykiss*) Bluegill sunfish (*Lepomis macrochirus*) Zebra fish (*Brachydanio rerio*)
Aquatic invertebrates	Daphnids (*Daphnia magna, Daphnia pulex*)
Aquatic crustaceans	Mysid shrimps (*Americamysis bahia*)
Sediment dwellers	Chironomid midges (*Chironomus riparius*)
Higher aquatic plants	Duckweed (*Lemna gibba, Lemna minor*)
Algae	Green algae (*Pseudokirchneriella subcapitata, Scenedesmus subspicatus*)
Honeybees	European honeybee (*Apis mellifera*)
Soil macro-organisms	Common brandling worm (*Eisenia foetida*)
Other soil dwelling arthropods	Springtails (*Folsomia candida)*
Other arthropods	Aphid parasitoid (*Aphidius rhopalosiphi*) Predatory mite (*Typhlodromus pyri*)

Species	Explanation
For ecotoxicological data the 'worst case' data has been selected unless it appears wildly out of character with the majority of studies published. We have chosen specific species and endpoints where ever possible to ensure a harmonised and balanced data set. In some cases endpoints other than these may be used, where this is the case the accompanying text will provide additional information.	
Mammals	acute oral LD_{50} and short term 90-day NOEL as mg kg^{-1} bw

Birds	acute oral LD_{50} as mg kg^{-1} body weight
Fish	acute 96-hr LC_{50} and 21day NOEC as mg l^{-1}
Aquatic invertebrates	acute 48-hr ErC_{50} and 21day NOEC as mg l^{-1}
Aquatic crustaceans	acute 96hr LC_{50} as mg l^{-1}
Sediment dwellers	96-hr LC_{50} and chronic 28-day NOEC static water only and sediment as mg l^{-1}
Higher aquatic plants	14-day EC_{50} as mg l^{-1}
Algae	acute 72-96-hr EC_{50} and 72-96-hr NOEC biomass / growth as mg l^{-1}
Honeybees	Lowest or contact and oral LD_{50} as ug/bee
Soil macro-organisms	14-day LC_{50} and chronic reproduction NOEC as mg kg $soil^{-1}$ dry weight
Other soil dwelling arthropods	various endpoints depending on availability as mg l^{-1}
Other arthropods	various endpoints depending on availability
Carbon & nitrogen mineralisation	% effects.

Quality Control and Management

Data management activities involve trawling for new or previously unidentified data. Evaluating its fitness-for-purpose, undertaking quality control activities and adding it to the database. The database and website are updated several times each week.

Data is sourced globally from published scientific literature and databases, manuals, registration databases and dossiers, company technical datasheets and research projects as described above.

Prior to entry into the databases data is subject to quality control. This is involves peer review, cross checking against other databases and data sources and, where doubt exists and the original reference is known, the original source is revisited and possibly the quality score (see below) adjusted.

Fitness for purpose is evaluated based on experimental conditions being appropriate for Europe, scientific protocols utilised, quality control findings and how recent the data is.

Data is then weighted 1 (low) to 5 (high) according to the confidence we have in that data. A low score does not necessarily indicate incorrect data but indicates we have not been able to obtain verification. Generally, as a guide the weighting scores are assigned according to the following:

1	Estimated data with little or no verification
2	Unverified data of unknown source
3	Unverified data of known source
4	Verified data
5	Verified data used for regulatory purposes.

However, confidence weightings may be adjusted if reason to doubt verified data exists or there is reason for greater confidence in an unverified value.

Once data has been accepted for inclusion into the database, data is extracted and transformed with respect to units. References are recorded and hardcopies filed.

For further details

Contact us as:

PPDB Management Team
Agriculture and Environment Research Unit
School of Life and Medical Sciences
University of Hertfordshire, College Lane, Hatfield, Herts, AL10 9AB, UK
Telephone: +44 (0)1707 284580
Email: aeru@herts.ac.uk