PPDB
BPDB
VSDB
December 2020

University of Hertfordshire Agricultural Substance databases

The history behind the databases

It is hard to believe but the PPDB has been around, in one form or another, for almost 25 years and can be traced back to 1996. This short document describes the rationale for the development of the databases and the major events and milestones that have happened since the project began.

Good quality, reliable pesticide data has always been in demand to support risk assessments of various kinds such as those used in regulatory processes and for environmental monitoring. Going back 30 odd years the demand was there but identifying reliable data was a significant problem particularly for interested parties outside of the manufacturer and regulatory worlds. Most data were generated by manufacturers and largely regarded as commercial-in-confidence. Submissions for regulatory approvals were also confidential. Data that were published in various scientific journals were available only as hardcopy, access was expensive and identifying a specific parameter was a time consuming and frustrating experience. At that time, and generally up until the early 2000s, researchers collated data and formed their own datasets. Each research project has its own database and, invariably the data was different from one database to the next. Not just in terms of the range of pesticides covered but also the parameters included, the metrics used and the actual data values. This was far from ideal as it meant that risk assessments done at different times with different input data could not be compared. Each new database meant time and money to develop it and once the project was complete there was rarely funding for the future management of the database. It was widely recognised that a single global, comprehensive database that was managed effectively was needed but, despite many different organisations trying, securing funding was a problem due to the global reach (so benefit) and long-term financial commitment needed. At that time 'impact' was not a parameter used to judge research success or value for money.

Whilst this debate was ongoing, in 1996, the University of Hertfordshire's Agriculture and Environment research Unit (AERU) began a research project on behalf of the UK Ministry of Agriculture, Food and Fisheries. The aim of the project was to develop prototype software to enable environmental assessments to be conducted on farm. This was a 'blue sky' type project as computers on farm were not common and awareness of the potential environmental impact of farming was not high. EMA (Environmental Management for Agriculture), as the software was known, included a simple pesticide risk assessment that used a scoring and ranking process that relied on an embedded pesticide database. In 1999 the pesticide risk assessment was significantly upgraded to take a meta-modelling approach and simultaneously the database was also expanded. The EMA software was quite successful and several thousand copies were used on UK farms up until the software's retirement in 2005.

In 2006 AERU were part of a large international consortium undertaking an EU Framework Project to development pesticide risk assessment models (FOOTPRINT). Part of the work that AERU did was to further development the EMA pesticide database for use with this project. This work involved expanding the database with data from the international partners and undertaking a comprehensive review and validation exercise. As a result, AERU began to receive more and more requests for copies of the database.

Gradually, as the internet became more and more mainstream, various pesticide databases began to appear. By the mid-2000s, whilst data were more accessible, they were still sparsely distributed and managed by organisations with their own specific aims and objectives. Some government departments published online systems containing useful data, but these were often limited to just the substances approved for use in that country, they rarely covered all parameters needed for comprehensive risk

assessments. Generally, management and updating of these system were often poorly resourced. In ten years, although there had been advances the initial problem of pesticide data accessibility had not be adequately solved. To help address this, and to ensure that the data driving the FOOTPRINT models was transparent, in 2007 the EMA database went online and was rebranded as the Pesticide Properties Database (PPDB). Access to the database was free to all, however, the issue of funding maintenance, updating and further development was still a problem and so the decision to licence off-line use and charge a fee was taken. This has remained the policy for the last 25 years and has generated enough funds, topped up by occasional consultancy activities and use of the database in other research projects, to enable us to do the work needed. Therefore, we have managed to keep the online system free of charge which we know has been invaluable to many, especially those in developing countries.

In 2012 the Danish Environmental Protection Agency (DEPA) engaged with AERU to discuss the use of the PPDB to support the pesticide tax they were developing. DEPA wished to use the data within the PPDB to support a Pesticide Loading Indicator. The indicator would reflect the significance of the impact from an individual pesticide on human health, environmental quality and ecotoxicity. Indicator values would be used to determine the taxable rate. As part of this work the PPDB was independently verified by industry experts and so gave us and end users confidence in the data. The PPDB continues to support the Danish pesticide tax today and similar environmental indicators elsewhere in the world.

The PPDB also supported a range of other regulatory activities. For example, the 2000 Water Framework Directive requires surface water bodies to have a good chemical and ecological status. Consequently, regular monitoring is vital to identify problems and to facilitate corrective action but knowing which pesticides to monitor for can be problematic. The PPDB database has been used to establish effective water monitoring programmes in several countries, for example Sweden and Turkey. It has also been used further afield, in California, USA to prioritise pesticides for surface water monitoring in both agriculture and urban areas.

Risk assessments have not stood still in time and have developed significantly in terms of scope and scientific complexity. This has inevitably meant that the PPDB has also had to expand and year on year new data has been added. For example, health and safety of farm operators has been a major concern and plant dissipation data is key data to support these assessments and this is now included in the PPDB. Similarly, the global loss of pollinator species has driven improvements in risk assessments particularly in considering wild bee species so the PPDB now includes data on wild bees as well as honeybees.

In the last 10 years the availability of biopesticides (including bacteria, viruses, plant-derived and animal-derived substances) has grown considerably and the type of data relevant to these substances can be quite different to those relevant to traditional pesticide chemicals. In addition, there was also the issue of veterinary substances as some were used in both crop and animal agriculture whilst some were only used in veterinary medicine. Again, the range of data needed in risk assessments were different depending on the application. The database itself was also becoming very large and, therefore, the decision was made to divide the database, mainly for presentation purposes, into three systems: the PPDB, BPDB (BioPesticides DataBase) and the VSDB (Veterinary Substance DataBase).

In 2017, AERU collaborated with the Cambridge Crystallographic Data Centre (CCDC) which allowed us to further enhance the PPDB data identification and structural information. Many of the pesticide molecules within the databases can now be viewed in 3D. We also have excellent working relationships with many pesticide manufacturers who, not only subscribe to our database, but also provide data.

This brings us to the present day. This year all three databases have had a presentation upgrade and the underpinning management software has also been enhanced. Global usage grows at an ever-increasing speed and this year the daily page downloads is typically between 10,000 and 14,000, or well over 2.5 million a year.

AERU, 2020