March 2024

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 well over 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-plus years ago 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 laborious. 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 had 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; these often being inherently variable. 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 cost 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 (MAFF). The aim of the project was to develop prototype software to enable simple 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 online. 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. General management and updating of these systems were often poorly resourced.

In ten years, although there had been advances the initial problem of pesticide data accessibility had not been adequately solved. In 2007, to facilitate this, and to ensure that the data driving the FOOTPRINT models was transparent, the EMA pesticide database went online and was rebranded as the Pesticide Properties Database (PPDB)[1]. 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 since its inception 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 2010 AERU collaborated with the International Union of Pure and Applied Chemistry (IUPAC) which resulted in IUPAC endorsing the PPDB and a IUPAC-branded version of the PPDB was launched.

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[2]. 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 including the UK Pesticide Load indicator[3,4] which is a modified version of the Danish system adapted for the UK's environment and general pesticide policy.

The PPDB has 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. Plant dissipation data is key requirement to support these assessments and this is now included in the PPDB[5]. 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[6]. In addition, ecotoxicity data for non-target beneficial insects has been expanded. More recently, in response to concerns regarding the risk to humans and biodiversity of air-borne pesticide pollution new parameters on volatilisation rates and photochemical oxidative degradation rates have also been added.

In the last 12 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 online 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. A recent collaborative exercise with industry enabled expansion, updating and validation of soil and groundwater metabolite data.

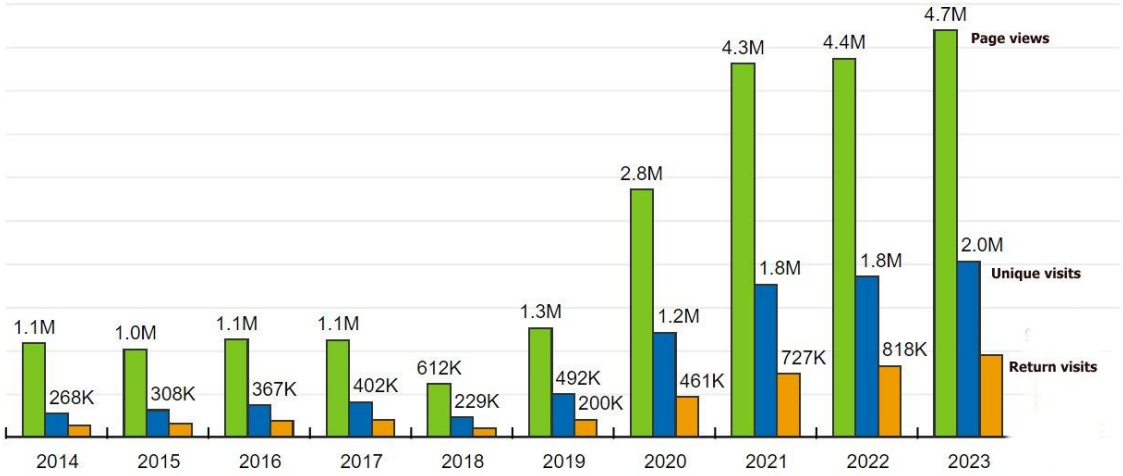

Figure 1: PPDB growth over the last 10 years

This brings us to the present day. As shown in figure 1 above, global usage continues to grow. This year the daily page downloads from the PPDB is typically around 14,000 on a normal working day equivalent to an approximate monthly average of 400K or close to five million a year (figure 2).

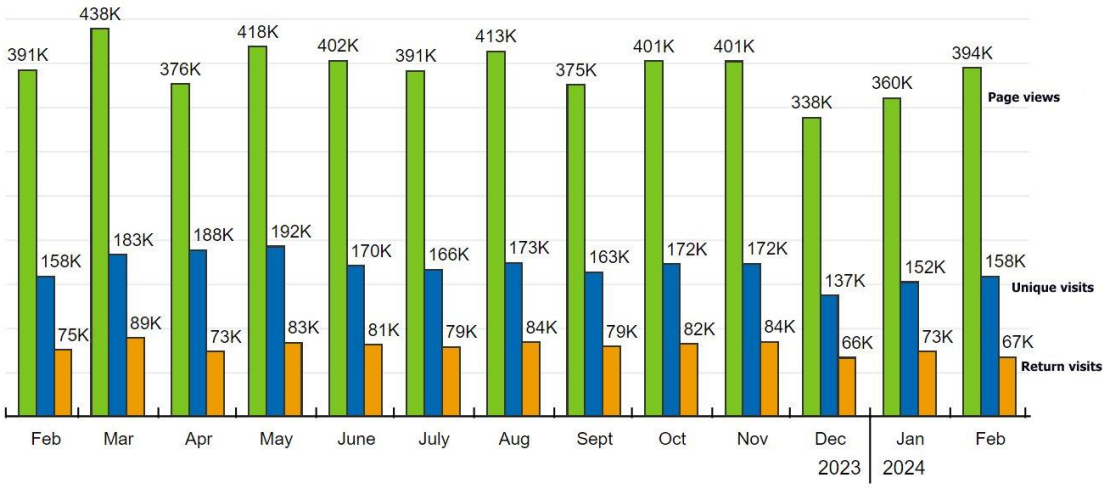

Figure 2: PPDB access over the last year

AERU, March 2024

References

1. Lewis, K.A., Tzilivakis, J., Warner, D. & Green, A. (2016) An international database for pesticide risk assessments and management. *Human and Ecological Risk Assessment: An International Journal*, **22**(4), 1050-1064. DOI: 10.1080/10807039.2015.1133242
2. Miljøstyrelsen (2012) The agricultural pesticide load in Denmark 2007–2010. URL: https://www2.mst.dk/Udgiv/publikationer/2012/03/978-87-92779-96-0.pdf (Last accessed: 03/04/24)
3. Lewis, K., Rainford, J., Tzilivakis, J. and Garthwaite, D. (2021) Application of the Danish pesticide load indicator to arable agriculture in the United Kingdom. *Journal of Environmental Quality*, **50**(5), 1110-1122. DOI: 10.1002/jeq2.20262
4. Rainford, J, Tzilivakis, J., Garthwaite, D., Jones, G. & Lewis, K.A. (2023) *Finalising a Pesticide Load Indicator for the UK: Phase 4 Report*. Prepared for the Department for Environment, Food and Rural Affairs (Defra), UK, for project PC0116, by FERA Science Ltd and the Agriculture and Environment Research Unit (AERU), University of Hertfordshire, UK. Available at: https://randd.defra.gov.uk/ProjectDetails?ProjectId=21074 (Last accessed: 03/04/24)
5. Lewis, K. & Tzilivakis, J. (2017) Development of a data set of pesticide dissipation rates in/on various plant matrices for the Pesticide Properties DataBase (PPDB). *Data*, **2**(3), 28. DOI: 10.3390/data2030028
6. Lewis, K.A. & Tzilivakis, J. (2019) Wild bee toxicity data for pesticide risk assessments. *Data*, **4**(3), 98. DOI: 10.3390/data4030098