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IMPROVED SSD SOFTWARE COMING SOON FOR THE ANZG GUIDELINES

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THE ADVENT OF BURRLIOZ

The rewrite of the 1992 Australian/New Zealand water quality guidelines (ANZECC 1992) in the late 1990s was predicated on a desire to move towards a more 'risk-based' approach to water quality assessment and management. Central to that effort was the replacement of subjective assessment factors (AFs) used in the derivation of 'safe' or 'protective' concentrations with the statistical device known as the Species Sensitivity Distribution (SSD).

By requiring mathematically simple forms for the SSD, the Dutch described how a log-logistic distribution could be fitted and an x% hazardous concentration (HCx) estimated using nothing more than a calculator (Aldenberg and Slob 1993). While the simplicity of this approach was appealing, it was also limiting in terms of the range of distributional shapes that could be accommodated. Accordingly, a small team of statisticians at CSIRO's Floreat laboratory undertook preliminary investigations into the use of more flexible probability models. One of us (Fox) had had experience with the Burr family of distributions in a totally different context and suggested that it might be equally useful for describing the distribution of toxicity data. As it turned out, this proved to be the case with the extra parameter of the Burr III distribution affording the flexibility sought. The Burr III had two other very appealing attributes: (i) the log-logistic distribution used by the Dutch was a special case of the Burr III distribution; and (ii) the closed-form of the cumulative distribution function (*cdf*) meant that HCx computations could also be done with a scientific calculator. The 'downside' was that estimation of the 3 parameters of the Burr distribution required the use of specialised software as it was both complex and computationally intensive. Although this posed no difficulties for statisticians, it did present a potential barrier to uptake by the ecotoxicology community.

The release of the Burrlioz 1.0 software coincided with the publication of the revised Guidelines in 2000 (ANZECC/ARMCANZ 2000). This was developed by CSIRO statisticians in Perth and was written in the Tcl language with the Tk toolkit used to develop the front-end GUI. Burrlioz was (and still is) only available as a compiled executable file for Windows-based machines. As an aside, the name Burrlioz was coined by co-developer Mark Palmer in CSIRO's Mathematical and Information Sciences (CMIS) Division. The name aptly conveyed both the statistical underpinnings and the nationality of the development team and was also a nod to one of Mark's favorite composers, Louis-Hector Berlioz.

A re-write of Burrlioz was commissioned by the Australian government in 2013 to take advantage of the computational and graphical elegance of the R programming language. Web-based deployment of Burrlioz was contemplated at the time but the decision was made to stay with the distribution of a compiled EXE program. This required a new front-end to be written to provide the interface between the user and the R language. And so Burrlioz 2.0 was released in 2014, again as a compiled download from the CSIRO website.

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LIMITATIONS OF BURRLIOZ

Burrlioz has been the workhorse of SSD modelling in Australia and New Zealand for over 20 years. While it has proved to be particularly good at modelling a wide variety of toxicity data sets, it has nevertheless continued to suffer from several drawbacks. Principally among these are: numerical stability issues with the Burr III distribution that can result in a failure to converge in the parameter estimation routines, with the consequential need to default to an alternative pre-specified distribution (inverse Weibull or inverse Pareto); lack of transparency – users cannot interrogate the code or make modifications; limited technical support; no software maintenance; and no bug reporting mechanism or process for fixing.

Perhaps the biggest limitation of Burrlioz, and one shared by most existing SSD fitting packages, is that it is limited to fitting only one distribution to the dataset. The limitations of relying on a single distribution are becoming increasingly clear. With toxicity datasets often being small (i.e. <15 values), it is not possible to statistically determine the best fitting distribution, assuming more than one distribution is even available to use. Although different distributions often give similar protective concentrations (PCs) for a toxicant dataset, there are exceptions for which the Burr III does not perform very well, especially at the PC99 level (i.e. 99% species protection level). In some cases, the Burr III produces a very long lower tail, resulting in very low PC99 values. Ideally, the Australian and New Zealand Guidelines (ANZG) require an approach that is less susceptible to dubious model fits.

AN IMPROVED APPROACH – SSDTOOLS AND MODEL AVERAGING

In 2018, a new SSD program known as shinyssdtools (comprising the R package named ssdtools and an accompanying web-based interface shiny) was developed by statisticians under contract to the British Columbia Ministry of Environment and Climate Change Strategy in Canada. In addition to being used by British Columbia, the use of shinyssdtools was also being considered at the national level by Environment and Climate Change Canada. The key feature of the ssdtools package is that it employs a technique known as model averaging. Model averaging is a statistical method for fitting several distributions (e.g. Burr III, Gamma, Log-Gumbel, Log-logistic, Log-normal and Weibull) to a (toxicity) dataset. Protective concentrations are estimated from the model-averaged SSD which is a weighted average of the selected distributions with the weights based on goodness-of -fit statistics. Thus, there is no longer a reliance on just a single model, regardless of whether or not it provides an adequate representation of the data. More details on model averaging are provided by Schwarz & Tillmanns (2019), Fox et al (2021) and Fox et al. (2022).

Following a 2019 workshop on the future of SSD modelling in Australia and New Zealand (Fisher et al. 2019; https://bit.ly/3d41Z6a), formal discussions were initiated with the Canadians on ssdtools and shinyssdtools. The resulting 3.5-year collaboration involving the Australian government (DAWE), AIMS, CSIRO, Environmetrics Australia, WQadvice, Environment and Climate Change Canada, Poison Consulting Ltd (CA), and BC Ministry of Environment and Climate Change Strategy, aimed to (i) further improve the statistical basis of ssdtools and (ii) assess its suitability for adoption as part of the ANZG (2018) Guidelines. A copy of the project's final report (Fox et al., 2022) is available for download at https://bit.ly/3TYN6T8. The project concluded that ssdtools represents a superior and more technically defensible SSD fitting approach than Burrlioz, and recommended that it be adopted in Australia and New Zealand. Notably, although Burrlioz and ssdtools often produce similar PC estimates, differences are sometimes observed owing to the ability of ssdtools to capture a wider range of distributional shapes than Burrlioz.

WHERE TO NEXT AND WHAT YOU CAN DO TO HELP

Consistent with the principle of continual improvement, the Guidelines' oversight committees have recently approved the transition from Burrlioz 2.0 to ssdtools and shinyssdtools. While Burrlioz has

provided a technically defensible approach to deriving toxicant guideline values for the past 20+ years, the benefits offered by a transition to shinyssdtools and the accompanying use of model averaging represents a significant strengthening of the technical underpinning of toxicant guideline values for Australia and New Zealand.

Currently, a transition plan is being developed to ensure that all the necessary aspects required to make the switch to (shiny)ssdtools are addressed. This includes, among other aspects, the required updates to the Warne et al. (2018) guideline value derivation method and associated guidance on the ANZG (2018) website, additional template requirements for default guideline value technical briefs, stakeholder communication/consultation regarding the transition, formalising hosting and maintenance arrangements, and further assessing functionality and user features of shinyssdtools. More details, including estimated timeframes, will be available in coming months.

In the meantime, one way that ecotoxicologists in Australia and New Zealand can help is to try out shinyssdtools in advance and provide feedback on functionality and features that might help to further improve the use of this tool for deriving guideline values. shinyssdtools is currently accessible via https://bcgov-env.shinyapps.io/ssdtools/. A shinyssdtools implementation team will consider this feedback as we move towards formally implementing the new tool. If not required prior to implementation, functionality improvements can still be made at a later stage. Feedback on shinyssdtools can be logged at https://ecotox.science/forums/forum/ssds/.

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