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A user-friendly software tool for DEB-TKTD model predictions

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Background

Toxicokinetic-toxicodynamic models based on dynamic energy budget theory (DEB-TKTD models) simulate sublethal effects of pesticides, exploring the effects of toxicants on growth and reproduction over time. DEB-TKTD models have great potential but are not yet ready for use in ERA (EFSA PPR 2018). The lack of user-friendly DEB-TKTD modelling tools was given as a major reason.

Now, we have developed DeEP (DEB-TKTD EP_x Predictor), a user-friendly, open-source software for making forward predictions with DEB-TKTD models.

Methods

- DeEP makes predictions relevant to pesticide ERA (specifically EFSA Tier-2C) for a species and compound of interest.
- DEBtox2019 model (Jager 2020) is used to predict toxic effects on growth, reproduction and survival (optional).
- Parameter estimation and validation must be performed beforehand.
- Predictions of the EP_x multiplier (see Box 1 for details) can easily be made for multiple environmentally relevant exposure scenarios.

Features

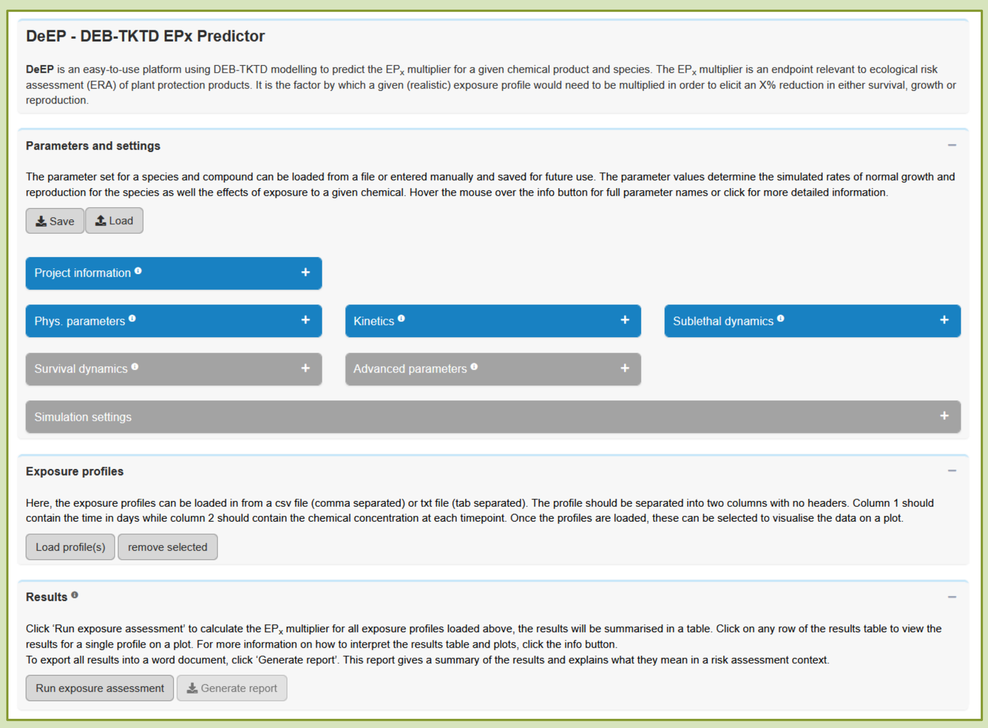

Figure 2: Screenshot of the user-interface

- User-friendly open-source tool developed with R shiny (shiny.rstudio.com).
- Browser version available online with source code published on GitHub.
- Project webpage provides background information, including user manual and quick start guide.
- User support and regular training courses (also on request): contact@deep-tox.info.

Box 1: Evaluation method

The software uses a 'Moving Time Window' approach to predict the 'EP_x multiplier' for a given chemical product and species.

Moving time window

- The exposure profile is broken down into overlapping time windows (Fig. 1) – predictions are made separately for each window.
- The length of the window may be the duration of lab studies or the lifespan of the species.

The EP_x multiplier

- EP_x multiplier = multiplication factor by which the concentrations (within a window) would need to be multiplied to cause X% effect (i.e. X% reduction in growth, reproduction or survival relative to control conditions).
- The higher the predicted EP_x multiplier, the lower the ecological risk posed by the chemical.

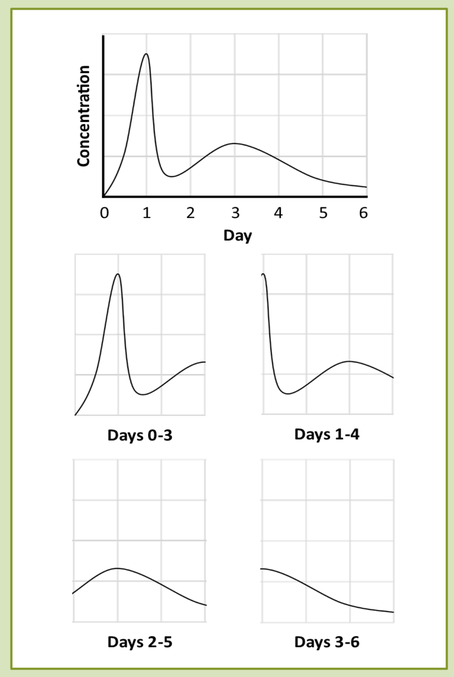

Figure 1: Example of a 6-day exposure profile broken down into four 3-day windows with 2-day overlap between consecutive windows.

Box 2: Overview of workflow

Parameters and settings

- Parameter set of a predefined DEB-TKTD model for a specific species & compound can be loaded from a file or entered manually and saved for future use.
- Descriptions of all parameters are easily accessible.

Exposure profiles

- Multiple exposure profiles, specifying external concentration over time, can be loaded and visualized (Fig. 3).

Results

- The software calculates the lowest predicted EP_x multiplier (growth, reproduction or survival) for each time window in an exposure profile and evaluates if the user-specified risk assessment criterion is met.
- Results are shown in a table and can also be viewed on plots showing the lowest EP_x for each time window vs the start of each time window (Fig. 4).
- Results can be exported in an automated report.

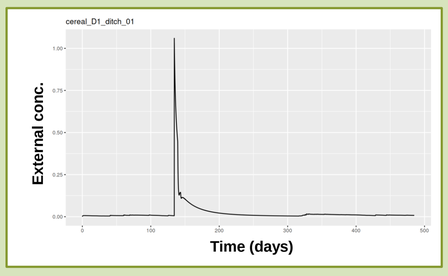

Figure 3: An example exposure profile as displayed in the software

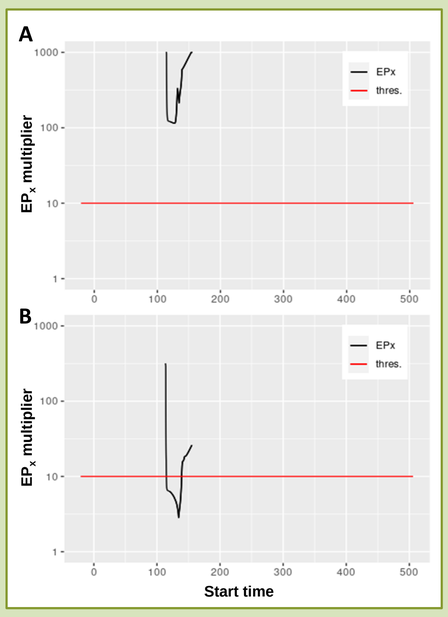

Figure 4: Results plots. Plot A is a pass while B shows a failure as the lowest EP_x multiplier (black line) is below the threshold value (red line).

Conclusion

- DeEP predicts the EP_x multiplier to be used in Tier-2C pesticide risk assessment.
- User-friendly and well-documented tool makes it equally accessible for non-experts and experts.
- Open-source publication and thorough documentation provide a transparent platform.
- **For more details visit our webpage: deep-tox.info**

https:\\deep-tox.info

References: EFSA PPR Panel (EFSA Panel on Plant Protection Products and their Residues), 2018. Scientific Opinion on the state of the art of Toxicokinetic/Toxicodynamic (TKTD) effect models for regulatory risk assessment of pesticides for aquatic organisms. *EFSA Journal* 2018;16(8): 5377, 188 pp. https://doi.org/10.2903/j.efsa.2018.5377.

Jager, T., 2020. Revisiting simplified DEBtox models for analysing ecotoxicity data. *Ecol. Model.* **416**, 108904, https://doi.org/10.1016/j.ecolmodel.2019.108904.