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Review

Dynamic energy budget models in ecological risk assessment: From principles to applications

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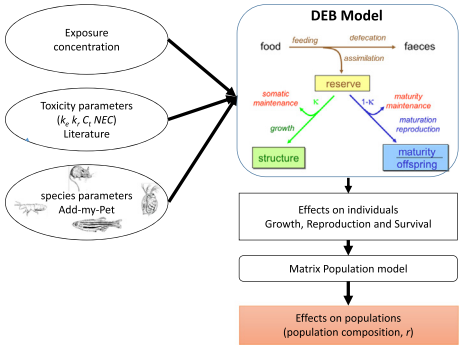
HIGHLIGHTS

- DEB theory is a framework for modelling time-specific lethal and sub-lethal effects.
- DEB models are promising tools for RA and have been applied to a variety of taxa.
- The Add-my-Pet database contains life cycle and DEB parameters for 857 species.
- Generic DEB models for RA are developed as open source tools as an EFSA project.

GRAPHICAL ABSTRACT



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ABSTRACT

In ecological risk assessment of chemicals, hazard identification and hazard characterisation are most often based on ecotoxicological tests and expressed as summary statistics such as No Observed Effect Concentrations or Lethal Concentration values and No Effect Concentrations. Considerable research is currently ongoing to further improve methodologies to take into account toxico kinetic aspects in toxicological assessments, extrapolations of toxic effects observed on individuals to population effects and combined effects of multiple chemicals effects. In this context, the principles of the Dynamic Energy Budget (DEB), namely the conserved allocation of energy to different life-supporting processes in a wide variety of different species, have been applied successfully to the development of a number of DEB models. DEB models allow the incorporation of effects on growth, reproduction and survival within one consistent framework. This review aims to discuss the principles of the DEB theory together with available DEB models, databases available and applications in ecological risk assessment of chemicals for a wide range of species and taxa.
Future perspectives are also discussed with particular emphasis on ongoing research efforts to develop DEB models as open source tools to further support the research and regulatory community to integrate quantitative biology in ecotoxicological risk assessment.

Abbreviations: AmP, Add-my-Pet; DEB, dynamic energy budgets; EFSA, European Food Safety Authority; LD_{50}, lethal dose for 50% of the individuals; LC_{50}, lethal concentration for 50% of the individuals; NOEC, No Observed Effect Concentration; NEC, No Effect Concentration; EC, effect concentration; EC_x, concentration with x% effect; ERA, ecological risk assessment; TK, toxico-kinetic; TD, toxico-dynamic.

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Contents

1. Introduction

Ecological risk assessment (ERA) of chemicals aims to characterise risks to the environment associated with chemical exposure combining an exposure and hazard dimension and to conclude on magnitude of effects that are deemed acceptable in relation to set protection goals (e.g. mortality). From a bird's eye view, frameworks for ERA often use tiered approaches which may depend on the aim of the assessment, the data available, and time-resources. For hazard identification and hazard characterisation, the first tier may use ecotoxicological endpoints from standardized laboratory experiments with aquatic and/or terrestrial species and at high tiers, results from semi-field to field trials. Using a first tier approach for hazard identification and hazard characterisation of regulated compounds (including pesticides and feed additives) assessments are often based on summary statistics like the No-Observed-Effect-Concentration (NOEC), Lethal Dose (LD_{50}), Lethal Concentration for 50% of the exposed individuals (LC_{50}) or 50% Effect Concentrations on growth (or growth rate) and reproduction (or reproduction rate) (EC_{50}) for a specified exposure time. Environmental quality standards are then usually derived using the lowest available summary statistics for the NOEC LD_{50}, $EC_{50,}$ applying an uncertainty factor (UF) to derive a predicted no-effect concentration (PNEC). The UF that is applied depends on data availability but in most cases it is the standard default value of 100-fold UF. This default value may be replaced by data driven UFs depending of data availability on taxa specific toxicity such as chemical specific adjustment factors (CSAFs) applied in the human health area (WHO, 2005).

Over the last decade, considerable research efforts have been put together to further improve risk assessment methodologies particularly to take into account mechanistic understanding of toxicity. In the human risk assessment area, the **Mode of Action** (MoA) framework has been developed by the US-EPA and WHO as 'a biologically plausible sequence of key events leading to an observed effect supported by robust experimental observations and mechanistic data'. MoA describes in a logical framework key cytological and biochemical events that are both measurable and necessary to the observed effect. MoA does not imply full understanding of **Mechanism of Action** (MeA) which relates to a detailed molecular description of individual biochemical and physiological key events leading to a toxic effect (Boobis et al., 2006; Meek et al., 2014). In toxicological terms, the MoA framework provides means to investigate toxico-kinetics (TK) and toxico-dynamic (TD) processes at different levels of biological organisation (organism, organ, cellular and sub-cellular level). TK describes the processes leading to the internal concentrations of a chemical or its metabolite(s) through knowledge of absorption (A), distribution (D), metabolism (M) and excretion (E) (ADME). TD describes the processes that lead to the toxic effects of a chemical or its metabolite(s) once it has reached the organ(s) or tissue(s) (EFSA, 2014). In ERA, a number of MoA classifications have been developed and include: 1. Verhaar classification using five broad categories based on general toxicological responses: class 1. Narcosis or baseline toxicity, class 2. Less inert compounds, class 3. Unspecific reactivity, class 4. Compounds and groups of compounds acting by specific mechanism, class 5. Unknown mechanism, 2. The U.S. Environmental Protection Agency (US-EPA) assessment Tool for Evaluating Risk (ASTER) MoA, 3. The US-EPA Mode of Action and Toxicity (MOAtox) database providing a high degree of specificity based on fish behavioural responses or weight of evidence classification (Kienzler et al., 2017).

The related concept of **Adverse Outcome Pathway** (AOP) emerged from the field of ecotoxicology and has been defined as 'a sequence of events from the exposure of an individual or population to a chemical substance through a final adverse (toxic) effect at the individual level (from a human health perspective) or population level (from an environmental perspective)'(Ankley et al., 2010). AOPs that have been investigated and depicted are available on the AOP Wiki tool (aopwiki.org). Recent reviews provide strategies, principles and best practices (Villeneuve et al., 2014a; Villeneuve et al., 2014b). The mapping of AOPs is a very active area of toxicological research and advances have been made to bring AOP together into networks. A recent review provided a description of an AOP network based on five reproductive and developmental toxicity-related AOPs for fish and illustrations on how such AOP networks can inform the development and refinement of laboratory assays (Knapen et al., 2015). Recently, (Teeguarden et al., 2016) have introduced the aggregate exposure pathway (AEP) as an intuitive framework to organize exposure data including ADME/TK data. The AEP framework supports, while making use of existing exposure models, the improvement of the generation, organisation, interpretation, modelling and prediction of data from exposure sciences including ADME/TK information (Teeguarden et al., 2016). In practice, the AEP also provides a holistic exposure counterpart to the AOP framework and a flexible tool to integrate the two frameworks together to apply risk-based, hazard-based, or exposure-based approaches in chemical risk assessment (Teeguarden et al., 2016).

In the food safety area, EFSA recently published a review on "Modern methods for human hazard assessment of chemicals" which focused on