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A review of key features and their implementation in unstructured, structured, and agent-based population models for ecological risk assessment

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The population-model database used for our statistical analyses and the codes are available in SI.

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Abstract

Population models can provide valuable tools for Ecological Risk Assessment (ERA). A growing amount of work on model development and documentation is now available to guide modelers and risk assessors to address different ERA questions. However, there remain misconceptions about population models for ERA, and communication between regulators and modelers can still be hindered by a lack of clarity in the underlying formalism, implementation, and complexity of different model types. In particular, there is confusion about differences among types of models and the implications of including or ignoring interactions of organisms with each other and their environment. In this review, we provide an overview of the key features represented in population models of relevance for ERA, which include density dependence, spatial heterogeneity, external drivers, stochasticity, life-history traits, behavior, energetics, and how exposure and effects are integrated in the models. We differentiate three broadly defined population model types (unstructured, structured, and agent-based) and explain how they can represent these key features. Depending on the ERA context, some model features will be more important than others, and this can inform model-type choice, how features are implemented, and, possibly the collection of additional data. We show that nearly all features can be included irrespective of formalization, but some features are more or less easily incorporated in certain model types. We also analyze how the key features have been used in published population models implemented as unstructured, structured, and agent-based models. The overall aim of this review is to increase confidence and understanding by model users and evaluators when considering the potential and adequacy of population models for use in ERA.

Keywords: Good modeling practice, ecological risk assessment, matrix models, agent-based models, ODE models

INTRODUCTION

The last two decades have seen substantial advances in the development of population models for the ecological risk assessment (ERA) of chemicals. These include guidance on systematic and consistent model creation and documentation (Grimm et al., 2020; Schmolke et al., 2017b), model evaluation and testing (Augusiak et al., 2014; Grimm et al., 2014; Schmolke et al., 2010b) and choosing models of appropriate complexity to address different types of risk assessment questions (Raimondo et al., 2018). A growing collection of case studies has clearly demonstrated how such models can inform risk assessment and risk management decisions (Forbes et al., 2016; Hommen et al., 2016), and slowly but surely there are indications that the acceptance of population models for risk assessment will continue to increase (EFSA, 2014; National Research Council, 2013). Nevertheless, there remains confusion about population models for ERA, including that related to differences among model types and the implications of including or ignoring different aspects of reality in the models. In addition, there is a lack of consensus on the role that the models should play in the ERA process.

Population models can be used to assess population-level effects over extended time periods, representing observed organism-level effects in an ecologically relevant context (Forbes et al., 2011; Hanson and Stark, 2011). While population models applied to ERA contexts share the objective to provide a tool for estimating long-term risks to populations, their underlying formalism, implementation, and complexity vary widely (Forbes et al., 2016; Grimm, 2010;

Raimondo et al., 2018; Schmolke et al., 2010a). Population dynamics can be formalized in models according to three basic types: unstructured, structured, and agent-based. These three types are mechanistic models, as they represent biological mechanisms underlying the structure and dynamics of populations. They differ from statistical, or empirical models, such as species distribution models (Elith and Leathwick, 2009), which are based on correlations.

Many characteristics of a species and its interactions with the environment can affect the structure and dynamics of its populations and, hence, also its responses to toxic chemicals. Key features that need to be considered irrespective of model type include density dependence, spatial heterogeneity, external drivers, stochasticity, life-history traits, behavior, energetics, and how exposure and effects are integrated in the models (see Table 1). In population models, they may be simplified, represented in great detail or not represented at all, depending on the specific purpose and scope of the model, the data available for parameterization and testing, but also on the familiarity of the model developers with different types of models. Depending on the problem at hand, some features are more important than others and could inform the choice of a model type. The absence of clarity and transparency about how to choose the key features to represent and the adequacy of different model types can increase skepticism towards population models.

Our goals are to provide an overview of the key features represented in population models of relevance for ERA, to clarify the differences among population model types, and define how they incorporate, or do not incorporate, these key features. We discuss the advantages and limitations of each model type and provide a perspective on the insights that can be gained by using different model structures and including or excluding various model features. We focus on the conceptual differences among model types but not on their formalisms in terms of equations or algorithms, which have been covered in earlier reviews of population models for ERA (Grimm, 2010; Schmolke et al., 2010a), or on details of parameterization and implementation, which are covered in textbooks and monographs about each model type (see references below).

Our overview is augmented by a statistical analysis of 450 population models published between 2004 – 2014 and compiled in a recent review (Forbes et al., 2016). In the review, models were categorized by model type and assessed with respect to features they represent. We evaluate these previously published models in terms of whether or not they include the key features of Table 1 and how inclusion is correlated with the three main model types. Our overview and analysis are intended to facilitate the systematic and efficient selection and evaluation of population models for use in ERA, and increase their understanding and use by risk assessors and risk managers.

We conclude that, as a result of their greater flexibility, ABMs are more amenable to the addition of all of the key features than are unstructured or structured model types *if* the data are available to do so. However, ABMs are more difficult to implement, analyze, and communicate than the other model types. Model complexity is not determined by model type, but rather by the number and type of features that are incorporated. The greater the model complexity, the more difficult a model is to implement and analyze, and the greater are the data demands. There is therefore a trade-off between the need to incorporate a particular feature, data availability and computational/mathematical effort that modelers have to take into account when using population models to answer specific ERA questions. When possible, we advise the use a multi-modeling approach, because it can increase confidence in model outputs to inform regulatory decisions.

MODEL TYPES

We distinguish three model types: (1) unstructured, (2) structured, and (3) agent-based models (ABMs). Other terms used are ‘scalar’ or ODE (ordinary differential equation) for unstructured models, ‘matrix’ for structured models, and ‘individual-based’ for ABMs, but we suggest using our terminology consistently in the future as it is non-technical and based on the key structural feature of each model type. Unstructured models ignore population structure whereas structured models do not, and agent-based models focus on the agency of individuals, in particular their adaptive behavior. Well-known examples of these model types are provided by Liu et al., (2005) for unstructured models, Caswell (2001) for structured models, and Grimm and Railsback, (2005) and Topping et al., (2009) for ABMs. The key aspects that distinguish the three model types are the kind of state variables they use to characterize a population and consequently, how demography, i.e., survival and reproduction, is represented.

In unstructured population models, the only state variable used is population size or total biomass. Any structure regarding, e.g., age, size, sex, or distribution in space, is disregarded. All these aspects are implicitly averaged over the entire population, and only the net outcome of survival and reproduction, the per capita population growth rate, is considered. It is possible in principle to add stochasticity to unstructured models, but this is rarely done for ERA because stochastic differential equations are much more difficult to parameterize, solve, and interpret than ODEs (e.g., Goel and Richter-Dyn, (1974)). Because population structure, spatial relationships and usually also stochasticity are not explicitly implemented in unstructured models, they include the implicit assumption that populations are large enough to disregard differences among individuals, space, and random variations (i.e., environmental and demographic stochasticity). In addition, unstructured model approaches imply that all interactions in the population are global, i.e. everybody equally affects, and is affected, by everybody else. For well-mixed populations, for example *Daphnia* populations in the laboratory, this assumption holds, e.g. (Martin et al., 2013), but for most real populations in the field it does not. Because of their limitations, unstructured models in an ERA context are mostly used as models of subsystems where their limitations are less relevant. Implementing unstructured models is straightforward. The well-established language of calculus can be used to clearly communicate the models, and standard software packages exist to solve the equations numerically (but see Seppelt and Richter (2005), on possible numerical artifacts). ‘Solutions’ in this case are the projected changes of population size over time, i.e., population size time series.

In structured population models, the state variables capture certain aspects of population structure such as age or stage. For example, for species with annual reproduction, numbers of individuals in each age class, ranging from recruits to the maximum achievable age, form a vector characterizing the structure of the population in a given year. Structured models represent the fact that demographic rates (sometimes called life-history traits) depend on age or stage, and demographic rates are averaged accordingly within each age or stage. Structure often matters. For example, a population of mainly old individuals will have a different growth rate, and respond differently to stress, than a population comprised of mostly young individuals. Most structured models are implemented by a set of linear difference equations, representing each class of the structure, for example each yearly age class. Each equation calculates the number of individuals in the next time step. The first equation, for class zero, includes the contribution to this class from all other age classes. Structured models are widely used in conservation biology, fisheries management and related fields, and are relatively popular in ERA (Forbes et al., 2016). Data from field surveys of populations are often recorded as age- or stage-specific numbers, which can be directly used to parameterize structured models. The population growth rate can easily be calculated and used as a comparative endpoint for risk assessment (Forbes et al., 2016, 2008). Additionally, structured models can include further features, such as density dependence or stochasticity, but then population growth cannot be calculated analytically, and population dynamics is simulated by updating the matrix of demographic rates in each time step and multiplying it with the current vector representing the population's structure. Structured models are easy to communicate and implement with existing software.

In ABMs, each individual is represented and may differ from all other individuals depending on its traits and behavior. Individuals are characterized by a set of state variables. In the simplest case this would only be age, and the ABM would be similar to an age-structured model. Usually, however, further variables are included because they are assumed to affect the individual's behavior, life history, and, in turn, survival and reproduction. ABMs are used when one or more of the following features are considered essential: (1) individuals are different, both within a population and over time as they grow and develop; (2) individuals usually interact locally, not globally; (3) individuals show adaptive behavior. Their decisions, for example about how to allocate energy to growth, maintenance, or reproduction, or when and where to forage, depend on what they know, what they want, and on the state of themselves and their environment. In ABMs, demographic rates thus emerge from agent interactions and/or the adaptive behavior of individuals rather than being imposed via, e.g., fixed survival rates or functions. Many ABMs are spatially explicit because they consider local interactions and the responses of individuals to local habitat features. Likewise, most ABMs are stochastic to represent variation that has been observed and is likely to be relevant, but for which mechanistic representation is considered infeasible or not necessary. ABMs have been used in ecology since about 1990. They are implemented as computer programs. In contrast to unstructured and structured models, which use the established language of mathematics and calculus, initially no established methods for formulating, implementing, or analyzing ABMs existed. However, the last decade has seen a maturation of such methods, including standards for model formulation and communication (ODD protocol, Grimm et al. (2020)), overall quality assurance (TRACE, Grimm et al. (2014); Schmolke et al. (2010b)), and systematic model analysis (Grimm and Berger, 2016; Thiele et al., 2012). Still, the range of complexity and the structural diversity of ABMs are much greater than those of unstructured and structured models. They are usually harder to develop, parameterize and analyze, but they are richer in structure and mechanisms, which makes them more realistic and easier to validate with various aspects of real systems (‘pattern-oriented modeling’, Grimm et al. (2005); Grimm and Railsback (2012)).

KEY FEATURES TO CONSIDER IN MODEL DEVELOPMENT AND EVALUATION

In this section, we provide an overview of key features that should be considered when developing, implementing and evaluating population models used for ERA: density dependence, spatial heterogeneity, external drivers, stochasticity, organism life-history traits, behavior, energetics and integration of exposure and effects. All these features are relevant for understanding population dynamics in general, and each of them has also been demonstrated in case studies to be relevant for ERA. Table 1 summarizes and briefly defines these features and illustrates that often the three main model types defined above can take into account any of these features. The following sections describe each feature in more detail by discussing their relevance for ERA, data needs, and whether and how they can be represented in the different model types.

Density dependence

Density dependence refers to variation in population growth rate with population size (Lebreton, 2009). It can be caused by different processes. The most common is when a resource is limited and individuals have to share it. Individuals may compete directly or indirectly for resources. In interference competition, individuals interact directly, often through aggression, to compete for a limiting resource, e.g., a territory. In exploitative competition, individuals interact indirectly by using up a common limiting resource, e.g., food or space. Competition may also be described as contest competition (in which the winner takes all and the loser gets none; e.g., territory, mate) or scramble competition (in which everyone gets less; e.g., food or space). Other sources of density dependence, such as cooperation and facilitation, can induce an “inverse” density dependence known as the Allee effect. In these cases, populations under a certain density threshold have a very low, or even negative, population growth rate, which can increase their likelihood of extinction (Courchamp et al., 1999; Pavlova et al., 2016). Hence, growth rate actually increases with increasing density. Allee effects can for example be caused by limitations in mating caused by low density, or any other social mechanisms that require a certain minimum density.

Relevance for risk assessment

Whereas it is expected that most populations in the field are under some form of density-dependent control (Moe, 2008), most ecotoxicological tests are performed under density-independent conditions in which test organisms are not constrained by limited resources. This is relevant for risk assessment because ignoring density dependence can lead to both over- and under-estimation of toxicant effects in field populations. For instance, compensation mechanisms can occur when populations under strong density-dependence are exposed to a stressor (Vaugeois et al., 2020): decreased density after exposure to a chemical reduces competition so that the remaining individuals may grow faster and bigger, and reproduce more. In terms of overall biomass or abundance, the direct negative effect of the stressor may thus be quickly compensated, but still lead to changes in population structure that affect risk (Gergs et al., 2013). Forbes et al. (2001b) reviewed experimental studies of density-toxicant interactions and found that some studies showed additive interactions between density and chemical effects on population growth rate, others found less-than-additive effects, and still others found more-than-additive effects. In at least one study, the form of the interaction varied across a chemical concentration gradient, with effects shifting from less-than-additive at low toxicant concentrations to more-than-additive at higher toxicant concentrations (Linke-Gamenick et al., 1999). Forbes et al. (2001b) were unable to identify simple, general a-priori predictions of the responses to toxicants of populations living under density-dependent control, which argues for explicitly incorporating density dependence in population models.

Incorporation in population models and data needs

There are two general approaches for incorporating density dependence in population models. The first involves making assumptions about the form of the density dependence and choosing a particular function to describe the relationship between population density and population growth rate (e.g., the Ricker Model, Ricker (1954)). The second approach involves incorporating rules for individuals to interact with each other or with the environment such that density dependence arises as an emergent property of the system.

Density dependence is usually included in unstructured population models by assuming that the population grows logistically until population growth rate is zero and density reaches a *plateau* (the habitat carrying capacity). Carrying capacities are inferred from observed equilibrium population sizes or from expert judgements or meta-analyses of the literature. Modifications of the logistic equation can also be found, e.g., to take into account the Allee effect. Density dependence can be added to structured models using a discrete time form of the logistic equation (Miller et al., 2002). This model is simple, because it does not require additional parameters or mathematical functions. If density dependence is known to act only on certain age or stage classes of the population (e.g. adult males competing for a territory), or if the strength of density dependence is likely to vary with stage or age, structured models can be used to incorporate such effects (Sable and Rose, 2008). This will require assumptions to be made about the carrying capacity of the population (Miller et al., 2002). In ABMs, similar approaches as in unstructured and structured models can be incorporated but are rarely used as they require the unrealistic assumption that individuals “know” the density of the population. In ABMs, density dependence rather emerges as a result of frequency-dependent interactions among individuals with each other or through the exploitation of simulated resources. Incorporating density dependence in ABMs requires that rules governing the behavior of individuals in the model be defined.

Density-dependence relationships are calibrated with laboratory or field data (Strauss et al., 2016). However, specifying density-dependent relationships from field data is very difficult (Lebreton, 2009; Sable and Rose, 2008). At the same time, if little is known about the strength or form of density dependence in a population, it may be misleading to assume an arbitrary functional relationship. For example, Raimondo (2013) showed that the functional form of density dependence can determine if toxicant exposure and density dependence are synergistic, compensatory, or additive. Thus, getting the functional form incorrect can dramatically change model outcome by influencing how density and toxicants interact. With ABMs it can be easier to represent density dependence, because for well-studied species sufficient data can allow the realistic representation of behavior and, hence, the emergence of density dependence (Stillman and Goss-Custard, 2010).

Model type considerations

Density dependence can be included in all model types. In unstructured and structured models this is usually done by adjusting a theoretical function, whereas in ABMs density dependence can be implemented as an emergent property linked to the rules governing interactions among individuals and influenced by environmental drivers. Letting density dependence emerge has the advantage that this can also be done for new conditions, which usually is not possible for imposed functional relationships.

Spatial heterogeneity

A model is deemed spatially explicit if it incorporates spatial heterogeneity and represents a landscape using cells (grids) or other approaches (e.g. networks of patches) (Dunning et al., 1995; Minor and Urban, 2007). The basic idea of "grid-based" models is that within each unit or cell, spatial relationships, e.g., the position of organisms, are ignored. This requires using a cell size that is small enough for this assumption to hold. If no such cell size can be found, e.g., because the organisms to be represented vary over orders of magnitude in size, grid-free approaches are used. Examples are the zone-of-influence approach for modeling plant populations and communities (e.g., IBC-Grass, Reeg et al. (2018)), or network-based models in which habitat patches are modeled as nodes in a network, and links between nodes represent possibilities for movement between them (Bodin and Saura, 2010).

Relevance for risk assessment

Organisms and environmental toxicants both exhibit considerable temporal and spatial heterogeneity (Spromberg et al., 1998). Therefore, representing spatial differences can be particularly relevant to study ecological processes that operate at different spatial scales, to explore different management strategies (Dunning et al., 1995), and to understand temporal and spatial heterogeneity of environmental toxicants (Spromberg et al., 1998). Spatially-explicit population models can increase the accuracy of exposure assessments and thereby support management decisions (Purucker et al., 2007). Moreover, it is valuable to consider spatial heterogeneity and take into account zones beyond the toxicant-contaminated area, because fluxes of organisms or materials functionally link the contaminated area to the surrounding landscape (Johnson, 2002).

Incorporation in population models and data needs.

By themselves, unstructured population models cannot deal with space, but if used as submodels of local habitat patches, they can represent space differences among different habitats. For example, one can divide space into two or more patches (or grid cells), each containing a population described by differential equations. These (sub)populations are characterized by their own abundance, survival, reproduction, and immigration/emigration rates and possibly other properties (Dunning et al., 1995). Mathematically, these models can represent the studied systems in two ways. One way is using a set of diffusion-reaction equations for each grid cell. They add a diffusion term, which represents random movement, to the ODE. Diffusion is driven by the difference in population densities between neighboring grid cells and used to calculate immigration or emigration rates (Spromberg et al., 1998). The other way is to use only one equation describing the change in the fraction of occupied patches over time (Maurer and Holt, 1996). Spatially explicit, unstructured models can be used to study dispersal and site-specific contamination, evaluate population persistence, or explore possible rules-of-thumb for predicting when a chemical exposure is likely to endanger the persistence of an entire population (Maurer and Holt, 1996). In structured models, space is taken into account using a similar logic as with unstructured models: sub-populations in different habitats are represented by separate matrices that are linked by functions defining migration between the sub-populations. The demographic rates combine demographic and dispersal information in potentially complicated ways (Hunter and Caswell, 2005). Usually, species' habitat and dispersal are included in stage-structured matrices using integrodifference equations, i.e., equations integrating both population demography and dispersal probabilities in a spatial domain (Lutscher and Lewis, 2004). Therefore, data on survival and reproduction rates and their spatiotemporal variability at different stages are required (Akçakaya, 2000). Since structured models are extensively used in conservation biology and species management, a substantial effort has been made to include spatial aspects in the models, despite the mathematical complexity of doing so. For example, RAMAS Landscape (Akçakaya et al., 2004) links a metapopulation model to the LANDIS landscape model, which is a forest succession model (Scheller et al., 2008). Agent-based models can easily take into account spatial heterogeneity, since each individual's location can be monitored (Topping et al., 2005). Such models can represent hypothetical or simplified spatial configurations (Ascensão et al., 2013; Purucker et al., 2007), describe a particular habitat in detail (Railsback et al., 2009), or be coupled with sophisticated landscape generators (Langhammer et al., 2019). Usually spatially-explicit ABMs are data demanding. However, if data are available, they can represent multiple spatial characteristics. Agent-Based Landscape Models (ABLM), for example, can include details about many processes, such as spatially-dependent animal behavior, food availability and accessibility, pesticide exposure and land management (Topping et al., 2005). When ABMs are supported by enough data, they can improve risk assessment by underlining the importance of factors such as the location of individuals in a population with respect to chemical exposure gradients (Liu et al., 2013). Nevertheless, simpler spatially explicit ABMs can also be useful in ERA (e.g., Purucker et al., 2007).

Model type considerations

Spatial heterogeneity can be included directly or indirectly within all model types. If data are rare or absent, unstructured models are a good choice since they can be used to study different spatial dynamics and thus guide future data collection and management decisions. If a fair amount of data is present and the modeler understands the complexity of particular mathematical constructs, structured models can be chosen. Available software can help model analysis, but this requires a deep understanding of the assumptions behind the software. If spatial data are available, and spatial heterogeneity and movement are supposed to influence many processes, ABMs are the best choice. They are mathematically less demanding and can potentially capture more spatially-dependent processes than the other model types.

External drivers

We define external drivers as any natural or human-induced factor that directly or indirectly causes a change in population size or structure and, hence, dynamics. External drivers can be chemical, physical or biological, and can affect an individual in different ways (activity patterns, energetic balances, physiology, etc.), eventually leading to an overall population response. They are major determinants of the structure and function of ecosystems, and may drive organismal adaptations that permit populations to persist (Barnthouse, 2004). External drivers can have a regular pattern (e.g. diurnal or seasonal) and therefore be easily predicted. Examples of such drivers are temperature, rainfall, tidal height, or fluctuating interspecific interactions. Other drivers are less predictable, such as fires, flooding or other extreme climatic events. Depending on the timescale of the study and the ecological and biological processes impacted by a stressor, external drivers might need to be included.

Relevance for risk assessment

Analysis of population trajectories is central to assessing risk in populations of concern (Alexander et al., 2009). External drivers can strongly modulate these trajectories, affecting different stages of an organism's life cycle and ultimately causing population-level fluctuations at various time scales (daily cycles or oscillations over multiple years). Some populations are much more influenced by external drivers than others. For example, for fish that overwinter, including seasonal environmental elements in a population model is critical and may give a very different outcome than assuming the population reproduces all year round. The dynamics of amphibian populations may be influenced by the availability of inundated areas and have very different dynamics in wet versus dry years. Consequently, exposure to toxicants may have different effects both at the individual and population-level depending on environmental fluctuations (Akçakaya et al., 2004). This may be especially important when considering impacts of climate change, since chemical stressors, temperature variability and related extreme climatic events may have complex and non-intuitive effects on organisms and populations. Determining whether and how to include external drivers in population models requires some basic ecological knowledge of the system under study (e.g., knowing how temperature influences different aspects of the life history), can be explored through the development of different model scenarios, and can be informed by sensitivity analyses (Raimondo et al., 2018; Schmolke et al., 2017b). Finally, external drivers can also have important consequences on the environmental distribution and toxicity of chemical pollutants (Noyes et al., 2009), as explained in the section **Integration of exposure and effects**.

Incorporation in population models and data needs

External drivers can be included in unstructured models by creating sets of equations and imposing rules, such as "if time equals t_x, then a fraction of the population is eliminated", or equivalently by expressing them as a set of equations representing different time periods (Barnthouse, 2004). In structured models, it is possible to take into account environmental drivers such as catastrophes, environmental variability or long-time cycles due to inter-specific interactions (Akçakaya et al., 2004; Carlson and Simpfendorfer, 2014). This can be adjusted *ad hoc*, by removing periodically a defined percentage of the population of particular age classes. Alternatively, vital rates of each stage can be multiplied by coefficients that change periodically, allowing the representation of population cycles (Akçakaya et al., 2004). Effects of random environmental variability can be expressed by probabilistically choosing among different transition matrices (Haridas et al., 2013) (see also the section on **Stochasticity** below). Matrix population models or models based on RAMAS/Metapop can also represent changes over time (and sometimes over space) of properties like carrying capacity or management strategies (Bagavathiannan et al., 2012; Meulebrouck et al., 2009). In ABMs, effects of external drivers can be added by modulating particular organism processes. For example, one can simulate temperature and/or food fluctuations and calculate their effects on individual metabolism at each time step (Accolla et al., 2019). Other environmental drivers can be hydrological variability and water turbidity (Focks et al., 2014b; Railsback et al., 2009), flooding (Schmolke et al., 2017a), or flowering periods affecting pollinator foraging (Becher et al., 2014). Alternatively, states of agents may vary according to a pattern defined by the day of the year or season. Data can come from actual environmental monitoring. Alternatively, one can use theories or rule-based criteria set by the modeler.

Model type considerations

External drivers can be theoretically incorporated in the three model types. However, in unstructured models this means creating a set of ODEs, instead of a single population model. Structured models and ABMs are more suitable for representing environmental drivers. Often, special rules need to be implemented to represent processes at different time scales. ABMs are particularly flexible in this regard.

Stochasticity

Stochasticity refers to random variations. Observed variations are referred to as ‘random’ if we do not know, or cannot know, the mechanisms underlying them. Examples are daily rainfall or temperature fluctuations, frequency of flooding or fires, etc. Conceptually, stochasticity (i.e., random differences) differs from variability (i.e., the extent to which values in a statistical distribution diverge from the average value and from each other) and from uncertainty (i.e., lack of knowledge about a value or process or measurement errors). However, in practice it is often not feasible to distinguish among these. Stochasticity, variability, and uncertainty in parameters, external drivers or other features of population models are often represented by drawing values from an assumed statistical distribution.

Relevance for risk assessment

Environmental conditions, such as good year versus bad year, can affect population growth rates and generate stochastic variation in population size. The greater the variability to which a population is subject, the greater the chances of going extinct (Tuljapurkar and Orzack, 1980). Stochasticity is even more important after a series of bad years that lead to small populations, which have a higher extinction probability. In a similar fashion, chemical exposure in the environment can be stochastic due, for example, to random rainfall or runoff events that drive input into nearby water bodies. Accounting for stochasticity may be crucial for ERAs given its potential influence on population dynamics and the responses of populations to chemicals and other stressors.

Incorporation in population models and data needs.

Including stochasticity in population models for ERA is helpful for quantifying the range of model output predictions regardless of model structure. This is usually done by randomly drawing variables from a probability distribution and iterating this process in every time step of the model projection. For example, if a survival probability is 0.3, a random number between 0 and 1 is generated and if it is larger than 0.3, the individual dies. The probability distributions can reflect the distribution of measured field data or can be defined *a priori* from probability theory (e.g., lognormal).

Unstructured models containing stochasticity are called SDEs (stochastic differential equations) instead of ODEs. These equations usually have one or more terms representing white noise or Poisson processes, but are relatively uncommon in ERA. In structured population models, stochasticity can be incorporated in the class-specific demographic parameters (e.g., death, birth and dispersal) by sampling different demographic rates from probability distributions at every time step. In ABMs, stochasticity can be included in multiple processes beyond mortality and reproduction (e.g., behavior, movement, physiology, inter- and intra- specific interactions). The number of stochastic processes accordingly depends on the model complexity, i.e., how many processes are represented that could include stochasticity.

Even though stochasticity is about random occurrences, an underlying knowledge of the frequency of such occurrences is important to generate reliable ERAs. As highlighted above, in practice it may be difficult to clearly distinguish stochasticity from variability and uncertainty. All of these contribute to the confidence (or lack thereof) in the resulting risk estimates. In general, the more processes to be represented in a model, the more opportunity for stochasticity, variability, and uncertainty to influence risk estimates, thus the higher the model's data demands. Because ABMs tend to include more processes than unstructured or structured models, data requirements, including those to capture stochasticity, tend to be greater.

Model type considerations

Stochasticity can be included in all model types. The inclusion of stochasticity means that unstructured and structured models cannot be solved analytically, but have to be solved by numerical simulations. The choice of probability distributions should be guided by data and knowledge about the stochastic processes irrespective of model type. Detailed methodology and code for the incorporation of stochasticity in models of different structure are available in (Caswell, 2008; Ellner et al., 2016; Grimm and Railsback, 2005; Morris and Doak, 2002). Current software packages such as RAMAS (for structured models) and VORTEX (for ABMs) greatly facilitate the incorporation of stochasticity.

Life-history traits

The life cycle of an organism refers to the sequence of events that occurs during the course of its development, starting with fertilization and ending with death. An organism's life cycle can be characterized by a series of life-history traits (including demographic or vital rates as well as qualitative features of the life cycle) that represent investment in survival, growth, and reproduction. They refer to individual-level traits and include age at first reproduction, time between reproductive events, lifespan, number and size of offspring, etc.

Relevance for risk assessment

The traits described above are important contributors to an organism's fitness, and for this reason are common test endpoints in ecotoxicology. In ERA, one is rarely concerned with protecting individual organisms, but rather populations and groups of populations (i.e., communities, ecosystems) (Hommen et al., 2010). Therefore, it is necessary to extrapolate the impacts of chemicals on individual life-history traits to population-level responses. Since the relationships between life-history traits and population dynamics are typically non-linear, context dependent, and vary among species, population models are needed to integrate them (Accolla et al., 2019; Schmolke et al., 2010a; Vaugeois et al., 2020). For example, the same percentage reduction in adult survival can have very different impacts on population growth rate for a long-lived species that produces few young compared to a short-lived, highly fecund species (Stark et al., 2004). Accordingly, toxic effects observed at the organism level can have very different implications for long-term population dynamics and persistence dependent on the species' life history (Forbes et al., 2001a; Forbes et al., 2019a; Martin et al., 2014). Currently, ecological risk assessments generally ignore the influence of life history and focus predominantly on individual-level toxicological sensitivity.

Incorporation in population models and data needs.

Unstructured models do not represent the life-history traits of the organisms, but generally use the intrinsic growth rate of the population *r*, which takes into account average birth and mortality rates. Structured models integrate information on demographic rates (i.e., stage-specific mean survival, growth and reproduction) to estimate population dynamics. Sometimes, structured models can integrate more complex physiological aspects or energetic theory (e.g. Klanjscek et al. (2006), see feature ‘Energetics’). ABMs usually incorporate individual survival/reproduction rates (e.g. calculating the probability of surviving or reproducing at each time step). These rates can change depending on the individual life stage (egg, juvenile, adult, etc.) if information is available. Life-history traits can also be implemented as resulting from more complex processes (see feature ‘Energetics’) or can be rendered variable between individuals in the population, for instance, based on their genetics (Bruggeman et al., 2010).

Because survival, growth and reproduction are the most common ecotoxicological endpoints measured, there are often data available from laboratory toxicity tests from control and chemically-exposed groups that can be used to estimate the relative change in these traits as a result of chemical exposure. Challenges can arise in obtaining relevant field data, particularly for inconspicuous life stages or age classes. For example, although fish are among the most frequently monitored taxa in the field, often there is no information on early life-stage survival, and it may be necessary to make some assumptions to fill in the missing data. This could be done using allometric relationships (e.g., relationship between adult body size and egg number) (Reiss, 1989), life-history theory (Stearns, 1992), or closely related surrogate species (Banks et al., 2010).

Model type considerations

Unstructured population models do not explicitly include aspects of an organism's life history. Therefore, this model type is not appropriate if it is of interest to incorporate life-history information, which often aligns with data measured in laboratory toxicity studies. In contrast, structured models require information on age- or stage-specific survival probabilities as well as fertility or reproductive rates at a minimum. Most agent-based models also explicitly incorporate life-history traits and aim to capture how these vary among individuals.

Behavior

Behavior is an organism's response to physiological and external biotic and abiotic factors. It is highly adaptable within genetic limits and therefore represents an important mechanism for how an organism reacts to environmental changes, including contaminants (Gerhardt, 2007).

Relevance for risk assessment

In the context of ERA, the role of behavior can be considered for both how it affects an organism's exposure to a stressor of interest and how it may be altered by stressor exposure. There are numerous examples of stressor impacts on the behavior of organisms in the context of ecotoxicological laboratory studies, which could lead to altered feeding patterns, movement speed and patterns (including local movements as well as migration), predator avoidance, aggression, etc., when considered in an ecological context (Chmist et al., 2019; Hedgespeth et al., 2014; Nabe-Nielsen et al., 2014). An example is avoidance behavior, which can be both driven by the stressor and impacts exposure to the stressor (Chaumot et al., 2003). Because behavior may influence organism exposure and response to a stressor, and stressors may cause sublethal behavioral responses that impact population dynamics, affected behaviors may be crucial to include in a population model.

Incorporation in population models and data needs

Behavior can only indirectly be incorporated in unstructured models. If one or more parameters depend on behavior, it is possible to create separate models (equal in structure but different in parameter values), and then compare the results. Preston and Snell (2001), for example, use a classical Lotka-Volterra model to study population growth in a predator-prey system of rotifers in the presence of a stressor affecting both reproduction and behavior (swimming speed). In this model, the prey-capture rate per predator depends on predator and prey swimming speeds, and can therefore change depending on the impacts of a stressor. Similarly, in structured models, behavior can indirectly be incorporated by the implementation of sub-models. Every sub-model is defined by its own stage-dependent properties (survival rate, fecundity, etc.), which can vary with external factors, such as stressor concentration and environmental properties. The links between these sub-models depend on behavioral dynamics. For example, toxicant-related behavior can be defined as a proportion of the population in a particular sub-model (or patch) that “decides” to move to another sub-model, characterized by a different environment and toxicant level (Chaumot et al., 2003). Behavior can be incorporated in ABMs directly, i.e., each individual behaves as in the real system. With this type of model, it is possible to take into account behavioral processes, such as mating, territoriality, nest building, as well as how toxicants affect those behaviors (Mintram et al., 2018). ABMs can also easily represent different spatial behaviors and the consequences of movement on exposure if the model is spatially explicit (Liu et al., 2013).

Behavior can be difficult to measure and quantify in a standard way across species, because it can take extremely diverse forms even if associated with similar life-history events (e.g. reproductive behaviors) (Hayward et al., 2012). To understand what behavioral considerations may be important for a population model, it is necessary to understand the role of those behaviors in the population dynamics of the species (e.g., the impact of predator avoidance on mortality rates), the impact of behavior on the exposure of an individual to the stressor (e.g., avoidance behaviors), and the consequences of stressor-induced behavioral changes on population dynamics (e.g., avoidance behaviors leading to less food consumption or impaired predator avoidance leading to higher mortality rates). Therefore, it is not possible to uniquely define the data needed to incorporate behavior as they are dependent on the particular behavior represented (different swimming speeds, probabilities to make a choice, mating strategies, stressor avoidance techniques, migration patterns, etc.), and how these activities interact with toxicant concentration and its spatio-temporal variability (see section on **Spatial heterogeneity**). Usually, specific laboratory experiments or field monitoring have to be performed to have a good parameterization of behavioral dynamics.

Model type considerations

Estimates of how an altered behavior may impact relevant endpoints (mortality or fecundity rates, predation rates, etc.) can be incorporated in any model type. However, unstructured and structured models offer limited possibilities to incorporate this feature. ABMs are particularly well suited, since they are designed to allow the simulation of individual behavior.

Energetics

Energetics is the branch of comparative physiology that quantifies the metabolic cost of various aspects of an organism's biological activity (Tomlinson et al., 2014). Usually this includes the energy required to fuel basal metabolic rate (BMR), standard metabolic rate (SMR), thermoregulation, growth, locomotion, reproduction, and any other set of activities that requires energy intake or consumption (Tomlinson et al., 2014). In the last decades, there has been a growing utilization of the concept of assimilated energy, both to determine organism growth and ecosystem productivity (Liao et al., 2006). The main reason for the growing appeal of energetic approaches is that they rely on the first principle of thermodynamics, i.e. the conservation of matter and energy (Beyers et al., 1999). Moreover, metabolism is one of the great unifying processes in biology, making connections between all levels of organization, from molecules to ecosystems (Brown et al., 2004).

Relevance for risk assessment

Organisms live in a fluctuating environment, often adjusting their energy use to stressful conditions such as resource limitation. If an additional pollutant-related stressor is present, the organism energy allocation may be impacted, likely causing a reduction in growth, reproduction or maintenance (Beyers et al., 1999). From an ERA perspective, understanding the energy budget of an organism can help to identify which metabolic process(es) is(are) affected by a toxicant (Kooijman, 2010; Sibly et al., 2013). Exposure to toxicants can be represented by a change in energetic parameters, such as a reduction in the assimilation of food or an increase in maintenance costs (Álvarez et al., 2006). The advantage of this approach is that the mode of action of the stressor can be better understood by analyzing which parameter change results in the best representation of data. For example, a reduction in reproduction can be caused by a stressor affecting different metabolic pathways. Depending on the mode of action, very different outcomes may result at the population level, even if the effect on individual reproduction is similar (Martin et al., 2014).

Incorporation in population models and data needs.

The energy budget of an organism, or of a group of organisms, is always represented as a balance between energy intake and expenditure. Energetics can be considered as a sub-individual module that is integrated more or less easily in different model types. The equations describing the different processes of metabolism (food consumption, growth, metabolic costs and waste products) can be empirically parameterized (Hanson et al., 1997; Pachzelt et al., 2013; Schmitt et al., 2013) or mechanistically calculated. Examples of empirically parameterized models include the Wisconsin fish model. Energetic models based on mechanistic theories (Sibly et al. ,2013) include the dynamic energy budget - DEB - model (Kooijman, 2010); the metabolic theory of ecology – MTE (Brown et al., 2004); the model for ontogenetic growth (West et al., 2001). Parametrization of any energetic model, whether empirically- or mechanistically- based, requires a large amount of information, e.g.

foraging, assimilation and growth efficiencies, allocation rules, physiological needs, morphological relationships, etc. (Emlen, 1989).

In unstructured models, energetics is represented by differential equations representing the change in biomass production of a population. Similarly, within structured models each class can be characterized by its own energetics and develops according to metabolic processes. Energy uptake and expenditure can be modeled as a function of age-specific or stage-specific body mass or age. Energy therefore drives the development of each class (Miller et al., 2011; Pachzelt et al., 2013). Other studies link more complicated energy budget models, such as DEB theory, to structured model parameters (Klanjscek et al., 2006; Klok et al., 2007). To do so, one must mathematically link the energetics model to stage-related survival and fecundity, solving complicated equations (see Klanjscek et al. (2006)). As for the other two model types, equation terms of energetically-based ABMs can be mechanistically explained (e.g. MTE or DEB) or defined operationally through measured (or measurable) changes in metabolic rates, most commonly through changes in measured respiration rate under different experimental conditions (Nisbet et al., 2012). Examples can be found in Jager et al. (2013); Schmolke et al. (2019).

Model type considerations

Energetics can be incorporated in unstructured, structured and agent-based models. They require a large amount of data to be adequately parameterized in any of the three model types, and the complexity of their mathematical formulation is mainly linked to the chosen energetic theory. Mechanistic theories usually result in more complicated equations, which have to be adapted to the specific model at hand.

However, these theories provide a common, codified framework to compare model results across different species and different levels of biological organization.

Integration of exposure and effects

The traditional risk assessment paradigm consists of problem formulation, exposure assessment, effects assessment, and risk characterization (Suter, 2007). Exposure and effects assessments are typically conducted in parallel, and then brought together in the risk characterization phase. At its simplest, this is in the form of a risk or hazard quotient in which a measured or predicted exposure concentration is divided by an effects concentration threshold (below which minimal effects are expected). In some cases, distributions of exposure and effects concentrations are compared with the area of overlap providing a probabilistic risk estimate.

Relevance for risk assessment

The entire purpose of ecological risk assessment is to relate the concentrations of chemicals to which organisms are likely to be exposed with those causing adverse effects to estimate risk. However, since the exposure and effects assessments are conducted independently, there is sometimes a mismatch that makes their integration challenging. For example, in aquatic systems, exposure to a pesticide may occur as a series of irregular peaks in time as a result of runoff events. This is then compared with the effects measured in a laboratory toxicity test performed under constant exposure concentrations and for a different duration than the relevant exposure duration in the field. This mismatch has to be addressed by ERA, especially with increasing evidence of climate-change driven alterations of environmental parameters, which affect the environmental distribution and biological effects of toxicants (Noyes et al., 2009). Population models can integrate exposure and effects on relevant spatial and temporal scales.

Incorporation in population models and data needs.

The link between exposure and effects is often implemented as a concentration-response relationship relating a particular toxicant concentration to an endpoint of interest (e.g. mortality rate). However, for temporally varying exposure scenarios, toxicokinetic/toxicodynamic (TKTD) models are the most appropriate tool for relating external exposure to internal uptake and organism-level effects. TK deals with the time course of the toxicant concentration in the organism, which changes because of absorption, distribution, elimination and biotransformation. TD deals with the processes that affect the organism at the toxicant target sites. TD models can be energetically based, describing the metabolic pathway that is affected by the toxicant (Ashauer et al., 2011). The General Unified Threshold model of Survival (GUTS) (Jager and Ashauer, 2018) has been developed to capture lethal effects, and DEB-Tox models (DEB models integrating sublethal toxicant effects) have been used as TD models. Incorporating spatially varying exposure scenarios into population models usually requires using a model that is spatially explicit (see section on **Spatial heterogeneity** above). Either monitoring data or fate model predictions are needed to characterize the exposure variability, and on the effects side, measurements of relevant effects at several exposure concentrations and/or durations will generally be needed.

Some unstructured models can describe exposure and effects through calculating an average mortality rate due to the exposure (Baveco et al., 2014) or through a TKTD model (Schmitt et al. (2013), see section on **Energetics** above).

Systems of ODEs (called non-autonomous ODEs) can also integrate variability in effects as a consequence of different exposure scenarios or toxicant dynamics. This involves the implementation of rules affecting, for example, demographic variables in response to pesticide application (Banks et al., 2008). This approach is already more efficient than using static dose-response assessments of toxicity, even if other model types can better incorporate effects over multiple generations (Banks et al., 2008). Structured models can integrate the effects that may occur during the various stages of the life cycle of an exposed organism by adjusting the stage- or age-specific demographic variables. Structured metapopulation models can take into account the spatial heterogeneity of exposure, but even without adding spatial complexity, these models allow characterization of the impact of a toxicant at the population level and over a longer temporal scale than can be tested in typical toxicity tests (e.g. Ducrot et al. (2007)). ABMs are increasingly used to integrate exposure and effects. Since ABMs can represent spatial and temporal variations without using complex mathematical objects, they can easily represent different spatial exposure and temporal scenarios. Such models have been used to test different exposure-effect scenarios and analyze the consequent changes in population dynamics and recovery patterns (e.g. Focks et al. (2014a); Galic et al. (2012)). Moreover, TKTD models are often used with ABMs (Ashauer et al., 2011).

Model type considerations

Although integration of exposure and effects are possible in any type of population model, ABMs are best able to incorporate the effects of temporally varying exposures, and spatially explicit ABMs and structured metapopulation models are well designed to incorporate effects of spatially varying exposures. The integration can be very simple (e.g., consider scenarios with different numbers and locations of clean versus contaminated patches in a metapopulation model) or very complex (e.g., overlay a GIS map of an actual landscape with realistic habitat features and actual field contamination data with a detailed simulation of individuals moving around the landscape and being exposed in space and time (Dalkvist et al., 2009)).

ANALYSIS OF PREVIOUSLY PUBLISHED POPULATION MODELS

We revisited an existing database of population models (Forbes et al., 2016) to investigate how some of the key features discussed above are associated with the different model types. Forbes et al. (2016) analyzed the frequency of incorporation of some features in population models from 403 peer- reviewed English- language publications published during 2004 to 2014. Reviewed publications described population models that have been applied to assess risks of pesticides to listed species or used in other contexts that could provide useful approaches and/or data for listed species risk assessments. In their review, the authors categorized models in terms of structure, taxonomic coverage, purpose, inputs and outputs, and whether the models included density dependence, stochasticity, risk estimates, or were spatially explicit. For the purpose of our study, we revisited the structure category, which had four attributes (Matrix, IBM, Unstructured, Multiple and Other), to match our three model types. Matrix was included as structured and IBM as agent-based. The Multiple and Other and the Unstructured categories were re-evaluated and included as appropriate. Moreover, we increased the number of entries to 450 because some studies included multiple model types. Our analyses extend the work of Forbes et al. (2016) by analyzing how some of the model features they assessed are associated with different model types.

Based on the information available in the database, we investigated the association between model type and the following six key features: density dependence, spatial heterogeneity, stochasticity, life-history traits, behavior, and energetics. We did not consider external drivers or the integration of exposure and effects, because these features were not present in the original database. We built contingency tables for each feature and performed Chi-square tests of independence to determine if there was a significant association between model type and each key feature. We then performed a Cramer's V test to determine the strength of the association. Finally, we performed a random forest analysis to understand which key features are the most important to distinguish the different model types. The modified database and details of the statistical analyses we performed are available in the SI.

Model types and key features

First, it is important to note that the database shows what key features have been included in models of the three types, not which key features they can or should include. Our analyses show that almost all key features have been included in all model types (life-history traits are not included in unstructured models), but that some features occur more frequently in some model types than in others (Figure 2). As indicated by the Chi-square tests, no features are independent of model type. For each feature, this means that the frequencies of inclusion in each model type are different than what would be expected from the overall frequency of this feature for all model types pooled. Density dependence has more often been included in ABMs (80% of ABMs in the database), whereas it has only been included in about 50% of the unstructured and structured models. ABMs are more often spatially explicit (more than 60%) than structured models (less than 45%) and unstructured models (less than

20%). Stochasticity has been included in the majority of models for all model types. About 90% of ABMs included stochasticity, whereas about 70% and 60% of structured and unstructured models included it, respectively. ABMs and structured models included life history in about 95% of cases. Behavior was included in about 10% of unstructured models, about 20% of structured models, and about 65% of ABMs. Finally, energetics was more often included in ABMs and unstructured models (10-20%) than in structured models (less than 5%).

The strength of the association (Cramer's V test) indicates which of the key features are more characteristic of certain model types, i.e. how different the frequency of inclusion of a feature is among different model types. The Cramer's V test does not specify which model type is associated with the analyzed key feature. The stronger associations were observed for behavior (Cramer's V test of 0.409) and life history representation (0.919). This means that these two features are most distinctive among model types. Density dependence (0.248), spatial heterogeneity (0.242), energetics (0.211), and stochasticity (0.191) are all less strongly associated with any particular model type.

We additionally analyzed the key features differentiating between model types using a random forest analysis. This method can be used to determine which variables (here: key model features) are the most important to consider in order to predict observations (here: model type). This analysis confirmed the previous results and underlined that life history and behavior are the two most distinctive features between model types. These key features are strongly associated with one model type (more represented in this type compared to the others), in our case the structured model type for life-history and the agent-based type for behavior.

Figure 3 presents the proportion of models of each type including a different number of the six key-features we considered for our analyses (from 0 to 6). The range of number of features is higher for agent-based models (from 2 to 6), whereas the ranges for structured and unstructured models are lower (from 1 to 5 and from 0 to 4, respectively). Moreover, most of the agent-based models include 5 features, which is more than structured (2 to 3) and unstructured (1) models. A straightforward but misleading conclusion would be that unstructured models are less complex than structured models, and that structured models are less complex than agent-based models. However, the number of features is not a proxy of model complexity, because some features can be more easily integrated in some model types than others. For instance, spatial heterogeneity and behavior can be more easily integrated in an agent-based model compared to an unstructured model. Consequently, an agent-based model that integrates these two features is not necessarily more complex than an unstructured model that only integrates one of these features. Therefore, model complexity is not only a matter of how many key-features are included, but rather related with how those features are included (i.e., to the mathematical formulation of the features and to their interactions with the other modeled processes).

DISCUSSION

In the last two decades, there have been multiple initiatives to increase the use of mechanistic models in ERA (Forbes et al., 2019; Thorbek et al., 2010). Chipps and Wahl (2008) recommended focusing on model evaluation, fostering interactions between model developers and model users, and reducing uncertainty in modeling applications for guiding management. Model documentation and evaluation are now widely recognized as important components of any modeling exercises (Grimm et al., 2020, 2014; Schmolke et al., 2010b), and communication between regulators and modelers is strongly encouraged (Forbes et al., 2019).

Many efforts have been made recently to promote the actual application of models as common practice in ERA, explicitly considering the perspective of risk assessors and managers. Raimondo et al. (2018) proposed a framework for developing and applying population models in regulatory decision making, expressly focusing on the regulators' perspective. Their work aims at defining the needs of models in accordance with the objectives of the risk assessment. Schmolke et al. (2017b) developed a systematic approach to transparently develop population models. The authors built a detailed decision guide that takes into account the available knowledge and data, and that is intended to help model development. Although this work explicitly targets modelers, its result is a communicable conceptual model that summarizes the decisions taken by the modelers. The conceptual model provides an excellent starting point for consultation with risk assessors and regulators prior to model implementation, to involve all stakeholder groups and ensure buy-in.

Our work builds on these earlier efforts and studies to assist risk assessors and managers in understanding the main types of population models, their advantages and limitations in association with specific ERA questions. Choosing the key features to represent in a model is part of the model development process and establishes the degree of complexity of the model. Decisions about model complexity depend on the model objectives, data availability, previous knowledge of the ecological system, and available resources (time, funding, etc.). The decision process related to considering key features, and deciding how they will be included in the model, leads to the creation of the conceptual model. The final conceptual model clearly states which features have been taken into account and should be discussed and understood by all involved parties before moving to the next step, i.e. model implementation. The model type is decided in this implementation step. As we demonstrate in the current review, the model type defines the underlying formalism of the model that can be adapted and extended to include representation of the key features.

Our work shows that the boundaries between the model types are sometimes blurred, since most key features can be included in unstructured, structured and agent-based models. However, some features directly inform the choice of model type. Density dependence, stochasticity, energetics and, to a certain extent, spatial heterogeneity are easily included in the three model types. Structured models and ABMs are more suitable for representing external drivers and life-history traits. Finally, ABMs are best able to incorporate behavior, effects of varying exposures and spatial heterogeneity, if the latter influences many processes.

As our overview shows, ABMs are the most flexible model type in terms of incorporating all key features in, if needed or possible, great detail. This comes to no surprise as unstructured and structured models aggregate information, which can limit how far the key features are taken into account. Still, the degree to which a key feature needs to be included, for example stochasticity or space, depends on the specific question and context. Furthermore, to include one or more of the key features in greater detail, ABMs need to be considerably more complex than the other two model types, which implies larger effort in terms of model building, parameterization, analysis, and application (Grimm, 1999). In practice, ABMs often would be “nice to have”, but constraints in data, time, or personnel can make it impossible to develop them in the time available. On the other hand, once an ABM including all key features, in particular behavior and bioenergetics, has been developed and tested, it can cover a wide range of questions and be adopted to new cases and systems (Stillman et al., 2015).

So far, the three model types discussed in this paper have been considered as exclusive alternatives, with clearly definable potentials and, in particular, limitations, as also shown by our analysis of previously published population models. Our work, coupled with systematic guidance on model development and implementation, prevents arbitrary model type selection, which can lead to ill-conceived statements concerning the relative merits of different modeling approaches for ERA (Bartell et al., 2003).

Insights from multi-modeling

The formalization and implementation of the conceptual model will depend on the model type chosen. As we show in our review, the formalizations of key features differ between model types. These formalizations come with advantages and disadvantages which may influence the model outputs (Meli et al., 2014). If the uncertainty about the model formalization is a concern for a particular ERA question, understanding and credibility of model results can be enhanced by a multi-modeling approach. Using a combined approach can add robustness to the conclusions drawn as well as highlight areas of uncertainty.

Examples from the literature show how using a multi-modeling approach can provide more insights to understand natural systems and model capacities (DeAngelis et al., 1993; Meli et al., 2014; Pagel et al., 2008; Pfister and Stevens, 2003; Topping et al., 2005). These authors compare ABMs with unstructured or structured models, showing that results are similar under many circumstances. However, under certain conditions, some factors can highly influence model outputs. For example, when using an ABM to model a population with positive temporal correlations in growth (i.e., individuals that grow faster than the mean one day, have a tendency to grow faster the following days), model outputs can diverge markedly from an unstructured model (DeAngelis et al., 1993). Similarly, population-level effects for different spatial distributions of a toxicant can be well represented by both ABMs and structured models in a homogeneous soil contamination scenario. However, predictions are not always consistent when contamination is heterogeneous, in particular if avoidance behavior and different food levels are included in the ABM (Meli et al., 2014). ABMs are therefore more suitable for risk assessment whenever fine-scale resolution, multiple stressors or particular behaviors clearly influence population dynamics (Meli et al., 2014).

These results stress the crucial importance of understanding which processes have to be taken into account when developing a population model for ERA. If results of different models are not comparable, this points to different assumptions taken during model conceptualization or different formalizations of processes in model implementation. The corresponding assumptions and processes can be identified as important in the context of the ERA (Topping et al., 2005). Therefore, we advise the use of a multi-modeling approach in some circumstances, because it can increase confidence in model outputs to inform regulatory decisions. For example, developing two models can increase trust in models for which full validation in the field is impractical. However, we acknowledge that this approach is sometimes infeasible because of budget or time limitations. This highlights once more how important it is that modelers, regulators and risk assessors understand and communicate about the whole modeling process, including the choice of the key features to represent, the model type to implement, and its assumptions.

CONCLUSIONS

In this review, we have provided an overview of the key features represented in population models relevant for ERA and a guide to understanding different model types, to clarify which insights can be gained by each of them. We have also analyzed how the key features have been used in published population models implemented as unstructured, structured (matrix), and agent- (individual-) based models. The review will help promote understanding of what the different model types are, how key features can be included in these model types, and how they drive the choice of model type. Our work joins the previous literature aimed at encouraging communication between regulators, risk assessors and modelers, and at ensuring the use of the best available science. It is meant to facilitate the efficient selection of population models for use in ERA, increase confidence in model conclusions, reduce subjectivity in model assessment, and enhance efforts in model evaluation.

Figures

Figure 1: Schematic representation of the three main model types. Each blue circle represents an individual and its radius the age, size or any other trait. The models represent the same wild population in three different ways. a) Unstructured models consider an average individual, without making any distinction among the organisms of the wild population. b) Structured models divide the population into classes (N_1, N_2, N_3), in which different organisms of the same age/stage/size are averaged. c) ABMs represent each organism, taking into

account as much individual variability as considered relevant (for more information see the text).

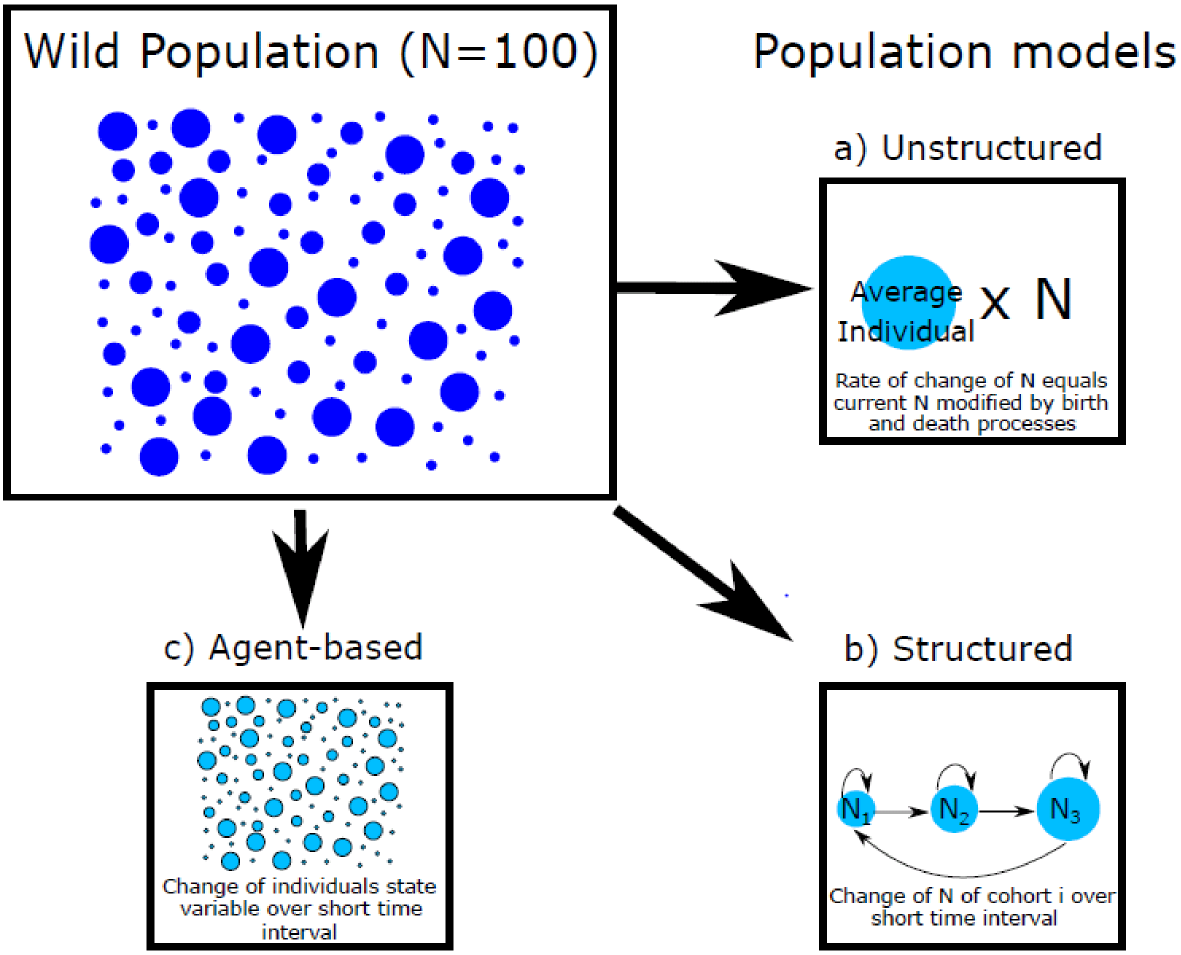

Figure 2: Summary of the statistical analysis of the model database compiled by Forbes et al. (2016). Each panel presents the frequency of inclusion of key features (y-axis, %) per model type (x-axis, Agent-based, Structured and Unstructured). The symbol (***) indicates the significance ($p<0.05$) of the Chi-square tests of independence. The different colors represent whether or not the feature was included.

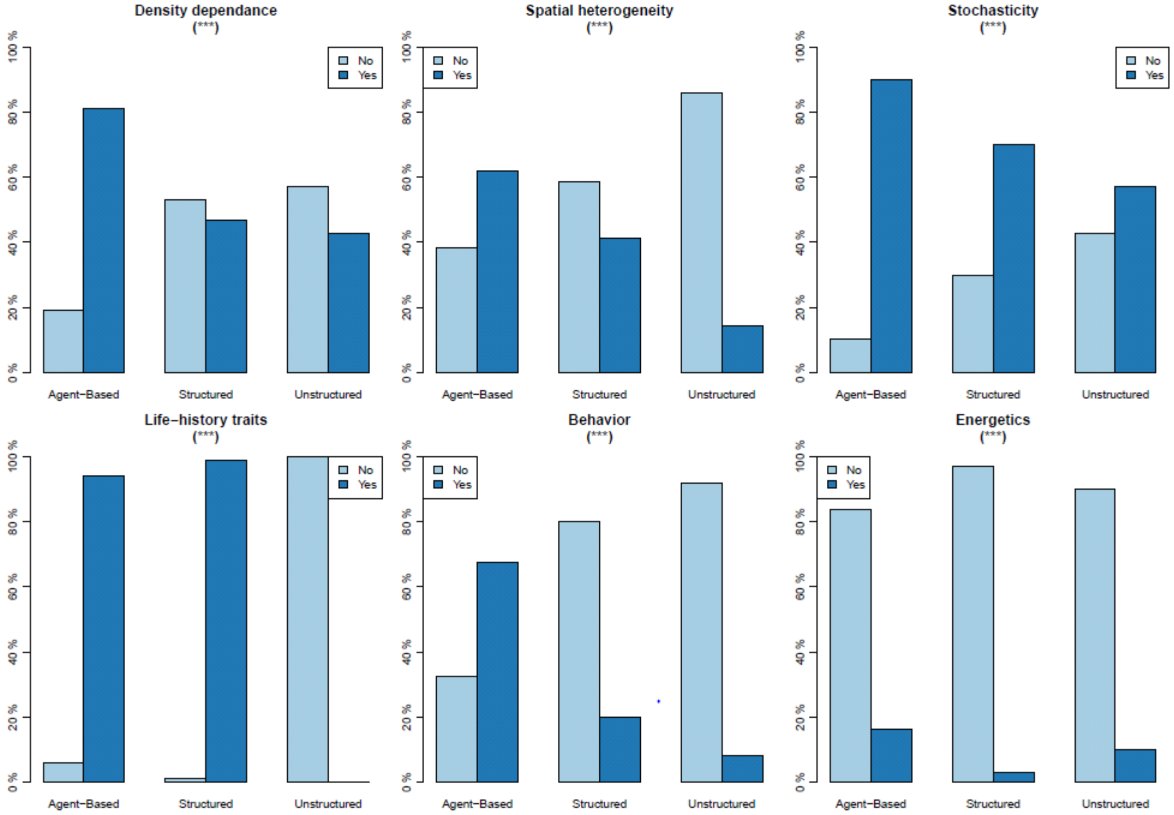

Figure 3: Proportion of models including 0 to 6 features for each model type. Each panel presents the proportion (y-axis, from 0 to 1) of models including a finite number of key-features (x-axis, from 0 to 6) for each model type (Agent-based in green, Structured in red, and Unstructured in blue).

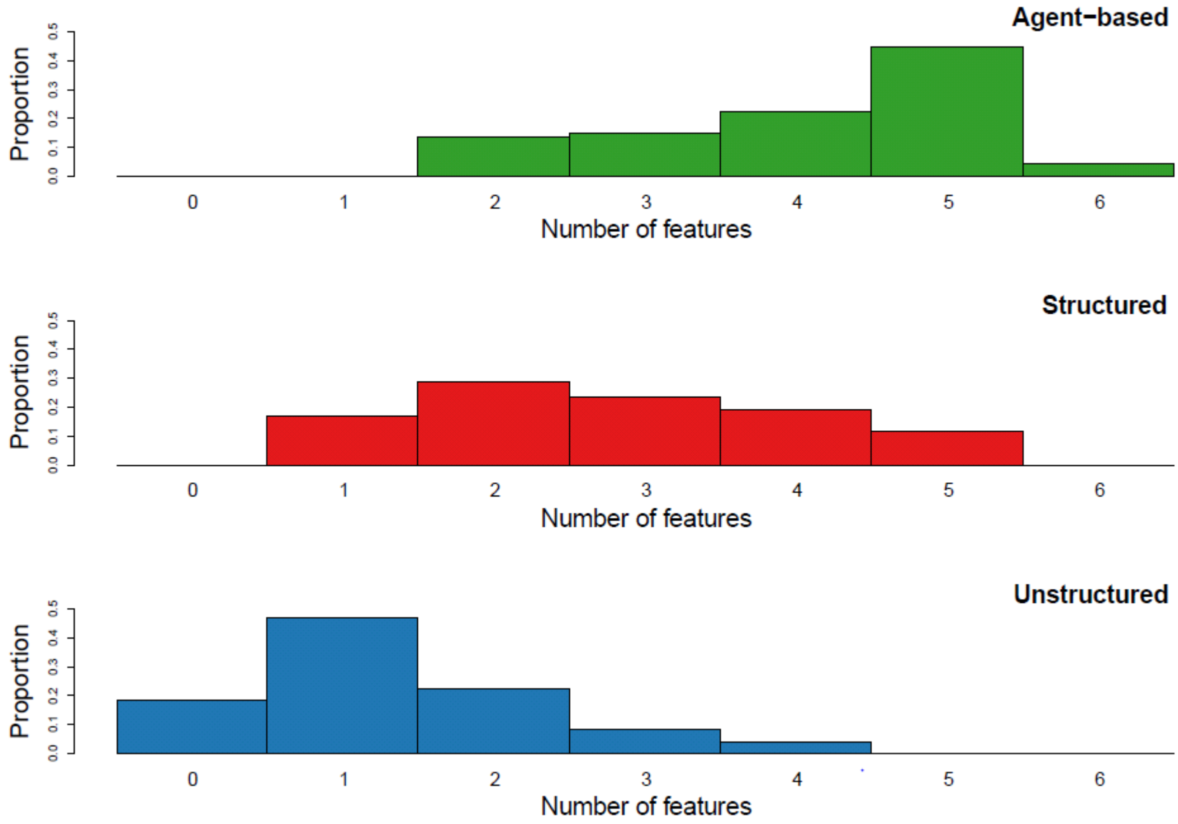

Table 1. Overview of key features to consider in the development and evaluation of population models for ERA.

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Table 1. Overview of key features to consider in the development and evaluation of population models for ERA.

Feature	Definition	How to include in population models			When to include
		Unstructured	Structured	Agent-Based	
Density dependence	Variation in population growth rate with population size due to competition	Describe population growth rate as function of population density. Usually represented by a logistic function	Describe population or stage-specific growth rate as function of population density (often logistic function)	Include rules governing behavior of individuals such that density dependence emerges	When resource limitation is expected to influence population dynamics (i.e. almost always) or populations are so small that Allee effects may be important
Spatial heterogeneity	Heterogeneity in biotic or abiotic habitat features that may influence organism performanc	Combine unstructured models as submodels, each representing a different	Represent connected habitat patches by different matrices (or other structured population	Represent continuous movement of each agent in hypothetical spatial configurations or using	When habitat variability is expected to have an important influence on organism behavior/fitness, exposure

	e and/or exposure to chemicals	connected habitat patch	representation)	real landscape data	to chemicals, management scenarios
External drivers	Temporal biotic and abiotic environmental changes that affect an individual's activity patterns, energetic balances, physiology	Use sets of equations and impose rules	Adjust demographic rates for different environmental conditions and impose rules	Use rules or functions to depict individual behavior in response to external drivers	When environmental fluctuations or changes are expected to influence population dynamics or exposure to chemicals
Stochasticity	Random variability in external drivers or organism properties or processes	Include a noise term to account for stochasticity	Draw demographic rates randomly from a probability distribution in each time step	Draw individual properties from probability distributions and use probabilistic rules for how to proceed in each time step	When it is important to quantify variation which is due to uncertainty in model outputs or provide probabilistic risk estimates
Life-history traits	Events in the life of an organism related to birth, survival, growth, and reproduction	Not represented	Use lab or field data to derive transition rates or theoretical relationships to predict transitions from one life stage to the next	Use lab or field data to estimate individual properties or processes or theoretical relationships	When (toxicity) data are available for survival, growth, or reproduction but the goal is to protect populations
Behavior	An organism's	Combine unstructur	Implement separate	Add agent behavior	When organism

	immediate response to physiological and external biotic and abiotic factors	ed models as submodels, each representing different behaviors	submodels with different stage-specific parameters	submodels using rules, functional relationships or decision algorithms	behavior is expected to have an important influence on chemical exposure or be influenced by chemical exposure
Energetics	Processes that involve energy intake, allocation, and expenditure (costs)	Use theoretical or empirical equations to represent the change in biomass production of a population	Use theoretical or empirical equations to characterize each stage or age by its own energetics	Use theoretical or empirical relationships to characterize energy gain and costs of each agent	When understanding the metabolic basis of changes in life-history traits influencing population dynamics or exposure is important
Integration of exposure and effects	Comparison of expected exposure to a chemical in space and time with the effects expected to occur at that exposure level	Represent exposure effects through parameters (e.g. mortality rate due to exposure) in the ODE, or in a system of ODEs that integrates variability in effects	Adjust stage- or age-specific demographic variables to defined exposure scenarios	Simulate different spatiotemporal exposure-effect scenarios acting on each agent using theory or empirical data	Always, as this is the central basis of ecological risk assessment of chemicals