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Authors: Valery E. Forbes[1*], Chiara Accolla[2], Thomas Banitz[3], Kristin Crouse[4,] Nika Galic[5], Volker Grimm[3], Sandy Raimondo[6], Amelie Schmolke[2], and Maxime Vaugeois[7]
[1]Department of Biological Sciences, Florida Atlantic University, Boca Raton, FL, USA
[2]Waterborne Environmental, Inc, Leesburg, Virginia, USA
[3]Department of Ecological Modelling, Helmholtz Centre for Environmental Research-UFZ, Leipzig, Germany
[4] Department of Ecology, Evolution and Behavior, University of Minnesota, St. Paul, MN, USA
[5]Syngenta Crop Protection AG, Basel, Switzerland
[6]United States Environmental Protection Agency, Office of Research and Development, Gulf Breeze, Florida, USA
[7]Syngenta Crop Protection LLC, Greensboro, North Carolina, USA
***E-mail contact:** veforbes@fau.edu

Conflict of interest

The authors declare no conflicts of interest.

Disclaimer

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Data Availability Statement

There are no data associated with this article. Detailed model descriptions and computer code for the reprinted conceptual model diagrams (i.e., Figures 1 - 4) are available through the original publications or by contacting the corresponding author Valery Forbes (veforbes@fau.edu)

Abstract: The use of mechanistic population models as research and decision-support

tools in ecology and ecological risk assessment is increasing. This growth has been

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facilitated by advances in technology, allowing the simulation of more complex systems, as well as by standardized approaches for model development, documentation, and evaluation. Mechanistic population models are particularly useful for simulating complex systems, but the required model complexity can make them challenging to communicate. Conceptual diagrams that summarize key model elements, as well as elements that were considered but not included, can facilitate communication and understanding of models and increase their acceptance as decision-support tools. Currently, however, there are no consistent standards for creating or presenting conceptual model diagrams, and both terminology and content vary widely. Here we argue that greater consistency in conceptual model diagram development and presentation is an important component of good modeling practice, and we provide recommendations, examples, and a free web app (pop-cmd.com) for achieving this for population models used for decision support in ecological risk assessments.

Key Points: Population models can be valuable tools for ecological risk assessment, and their use is growing together with improvements in modeling guidance. Communicating key features of complex population models to different stakeholders can be challenging. Standardization of conceptual model diagrams can facilitate model communication, evaluation, and acceptance. We propose a standard template and free web app for creating conceptual model diagrams for population models used to support ecological risk assessments.

Keywords
mechanistic effect models, Pop-GUIDE, good modeling practice, popcmd.com, model visualization

INCREASING USE OF AND GUIDANCE FOR POPULATION MODELS IN ECOLOGICAL RISK ASSESSMENT

The use of mechanistic population models as research and decision-support tools in ecology and ecological risk assessment (ERA) is increasing. For instance, recently updated European guidance documents for the risk assessment of pesticides to bee pollinators (EFSA 2023a), as well as to birds and mammals (EFSA 2023b) explicitly recommend the use of population models as higher-tier tools for risk refinement. In addition, a key Scientific Opinion on the use of mechanistic effect modeling for pesticide risk assessment in the EU (EFSA 2014) has played an important role in the growing acceptance of population models for decision support in ERA. In the USA, population models are suggested as ideal tools to be used in Step 3 of the harmonized risk assessment approach for species listed as threatened or endangered under the Endangered Species Act (ESA) (NRC 2013).

Growth in the use of population modeling for ERA has been facilitated by advances in technology that allow for the simulation of more complex systems, guidance on model evaluation (Grimm et al. 2005; Grimm and Railsback 2012), documentation (Grimm et al. 2006; 2010; 2014; 2020; Schmolke et al. 2010a), and development (Raimondo et al. 2018; 2021; Schmolke et al. 2017), as well as publication of targeted case studies (Hommen et al. 2015) and reviews of existing population models developed for risk assessment (Galic et al. 2010; Schmolke et al. 2010b; Forbes et al. 2016; Accolla et al. 2021). Forbes et al. (2016) identified a total of 403 population models published between 2004 and 2014, with about a quarter of these including some type of chemical stressor.

The guidance that has been developed over the last decade or so has greatly improved consistency in model documentation and description (e.g., Overview, Design concepts and Details (ODD) protocol, Grimm et al. 2020); TRAnsparent and Comprehensive Ecological modeling documentation (TRACE), Grimm et al. 2014), has facilitated model evaluation (Grimm and Railsback 2012; Gallagher et al. 2021), and has improved documentation and standardization of the model development process (including decisions about what not to include; Raimondo et al. 2021). Guidance on model evaluation, sensitivity and uncertainty analysis is also available (EFSA 2014). These tools are complementary and, when used together, greatly improve the consistency, transparency, and reproducibility of population models for use in decision support.

Yet, communicating population models to decision makers, such as government regulators, and other stakeholders (e.g., NGOs, general public), in a way that is easy to understand and that instills confidence in the models, remains challenging. At first glance, population models often look very different from each other, so that the impression can be given that each is unique and must be judged on a case-by-case basis. However, the models are often conceptually very similar, as they typically consider the same or similar aspects of a population. The differences come about because the building blocks are different depending on, for example, the specific question, data availability, and the species considered. It would therefore be desirable to have a graphical scheme, or conceptual diagram, that illustrates the commonality of the models, but is flexible enough to show differences.

The common aspects of populations to be considered imply that model development should follow a standard series of questions. Accordingly, the Population modeling Guidance, Use, Interpretation, and Development for Ecological risk assessment (Pop-GUIDE; Raimondo et al. 2021) was developed specifically for population models used in ERA. Pop-GUIDE is applicable across regulatory statutes and risk assessment objectives. It takes users through a standard series of questions that help model developers and risk assessors decide which features and processes to include in a model based on the model's purpose, as well as data and resource availability. Pop-GUIDE has been recommended in the most recent EFSA Bird and Mammal risk assessment guidance (EFSA 2023b; pp 105-106), and a number of case studies demonstrating the use of Pop-GUIDE have been published in a special issue of *Ecologies* (https://www.mdpi.com/journal/ecologies/special_issues/Population_Modeling_ERA#published)

In other fields, such as hydrology, standards for visualizing models have been suggested (Wang et al. 2021); this is not the case for population models. A standard visual overview would allow modelers to present their models in a way that is simple and general enough to be quickly grasped by non-modelers, and specific enough to provide a sufficiently detailed overview of a model's inputs, structure, and outputs. Our goals in this manuscript are to provide such a scheme, demonstrate it with a few worked examples, and introduce a web app designed to automate the generation of such diagrams for maximum consistency.

CONCEPTUAL MODELS AND CONCEPTUAL MODEL DIAGRAMS: CURRENT STATE OF PRACTICE

It is widespread practice to summarize population models using a so-called conceptual model, defined as "a high-level, graphical and textual summary of the components and functions within a model and their linkages" (Raimondo et al. 2021). The verbal description is often summarized in a conceptual model diagram (CMD), the purpose of which is to facilitate communication of the model to a variety of audiences. CMDs depict the relevant aspects of the model, with the details of sequences, conditions, and state variables described in an accompanying narrative. Table 1 provides an overview of the types of elements that are typically included in CMDs (see also Wang et al. 2021).

Conceptual model terminology and representation vary widely in the literature. Banitz et al. (2022) reviewed common visualization approaches for identifying and communicating causal relationships in complex social ecological systems and note that there is a lot of variability. Some of the alternative terms that have been used for CMDs include process diagrams (e.g., Hazlerigg 2019), overviews (Becher et al. 2014), schemata (Beaudouin et al. 2008), or state transition diagrams (Thorbek & Topping 2005). Some models are depicted as flow charts that start with the initial conditions, end with model outputs, and show a linear sequence of information or events in time during a model run (e.g., Giacomini et al. 2013; Meli et al. 2013; Figure 1).

In other cases, models are depicted as schematic overviews containing state variables, key processes, and external drivers, without including information on the flow of events during a model run (Girard 2014; Schmolke et al. 2017; Figure 2). Grimm et al. (2020) provides a “visual ODD” (Figure 3) that shows an overview of the entities and how they are initialized (“Initialization”), the processes and their scheduling (“Submodels”), and the observation, i.e. the key model output that is used for addressing the question of the model (“Analyses”).

This lack of consistency can make it challenging for decision makers to quickly understand what is included in a particular model and how to determine whether the model will make a useful contribution to their decision-making process. Moreover, the way that we visualize models of complex systems generally affects our understanding of them and the conclusions and decisions we can derive from this understanding (cf. Banitz et al. 2022; Sheredos et al. 2013). It has also become apparent that stakeholders want to know what features were considered, but ultimately not included in a particular model. Therefore, it is important that the CMDs provide a generic overview of the model elements, structure, and processes of a population model.

To be adopted, any guidance will need to be acceptable to both modelers and model users. Since CMDs are often provided the first time a new model is published, they serve as a critical communication tool that may influence whether or not the model is well-received by potential users. Similar to the Overview part of the ODD protocol (Grimm et al. 2020) they should provide a comprehensive overview of the model that allows relating models to other models, and that provides a roadmap for further reading about, or scrutinizing, a model. Well-designed CMDs can facilitate recognition of models, and this familiarity can improve user confidence and their understanding of what the models do. Thus, there is a need to have CMDs that are easily comprehensible to a range of stakeholders having different degrees of modeling expertise. Standardization of CMDs can facilitate their comprehension and allow different models to be compared more easily.

EXTENDING GOOD MODELING PRACTICE BY STANDARDIZING CMDS

As noted above, Pop-GUIDE (Raimondo et al. 2021) provides comprehensive guidance on the steps needed to create conceptual (population) models for use in ERA. However, it stops short of providing explicit guidance on how exactly to visualize such conceptual models. In the interest of clarity and consistency in how population models used for ERA are communicated, we here develop this next piece of guidance. Building on Pop-GUIDE and related guidance on Good Modeling Practice (EFSA 2014), we consider what key elements of mechanistic population models should be communicated in a CMD, suggest how these can be communicated clearly and consistently, and apply our recommendations to models of different structure and complexity to demonstrate how the approach could be applied in practice. We believe that an ideal CMD should be quick and easy to interpret, providing enough detail for readers to understand what key features and processes are, and are not, included in the model. Therefore, we built our CMD as a visual complement to the ODD protocol of Grimm et al. (originally developed in 2006 and updated in 2010 and 2020), and in particular to the Overview section of ODD. The ODD protocol standardizes the way that population models are described with the aim of providing a consistent, logical, and readable account of the structure and dynamics of population models. Although ODD was originally developed to describe agent-based models (ABMs), it has subsequently been applied to other model structures, has been shown to be useful in model design, and can also be used as a checklist when developing a model (Grimm et al. 2020). The first component of ODD, Overview, provides a description of the purpose of the model and patterns that it is designed to reproduce; a brief description of the entities, state variables, and scales of the model; and a process overview and scheduling. The remaining parts of ODD, Design Concepts and Details, go into more depth in describing various aspects of the model.

To determine what potential components of a population model should be considered for inclusion during model development and visualization, we build on the work of Accolla et al. (2021) which provides an overview of the key features of population models used for ERA. We follow Accolla et al. (2021) in categorizing population models into three types (unstructured, structured/matrix, and agent-based) and depicting the key features to consider for inclusion in the models (density dependence, spatial heterogeneity, external drivers, stochasticity, life-history traits, behavior, energetics, and integration of exposure and effects) based on model objectives. However, using only those elements, as shown in Figure 4 reprinted from Vaugeois et al. (2022), essential information is missing to understand the basics of how a model works (i.e., transition between stages, where the stressor or external factors act). Consequently, we combine those elements with other elements already present in Pop-GUIDE. Our intention is to provide a way to clearly communicate model structure and core components, which can often get lost in other details. Our overall goal is to facilitate communication and increase the consistency, transparency, and reproducibility of population models, in particular the way that they are visualized, to improve their value and increase their use as decision-support tools.

MOVING TOWARD A STANDARDIZED APPROACH FOR CMDS

The following represents a first attempt to standardize CMDs for population models used in ERA and demonstrate them by creating CMDs for two previously published population models for the decurrent false aster, *Boltonia decurrens*, (Schmolke et al. 2017) and fathead minnow, *Pimephales promelas* (Raimondo et al. 2021). We anticipate that details will change and improve as the standard template gains acceptance by users.

As defined by Accolla et al. (2021), the text boxes shown on the left panel of Figure 5 capture the key features generally considered for inclusion in population models. Because the key features encompass the potentially relevant components that need to be considered for population models in ERA, they can act as a checklist to ensure that nothing important is overlooked. Those features that are not included in a particular model will still appear in the left panel of the CMD, however, they will be grayed out to make it clear that they have been considered but not included. Following Pop-GUIDE (Raimondo et al. 2021), the accompanying text describing the model should provide an explanation as to why certain features were not included.

Through the use of categorical color palettes, we distinguish different types of model features. Green represents aspects of the environment, particularly any external drivers (including chemicals) that may influence population dynamics. For example, in the aster CMD (Figure 6a), external drivers include seasonal flooding regime and herbicide (i.e., atrazine) exposure. In the fathead minnow CMD (Figure 6b) external drivers include variability in juvenile overwinter survival and insecticide (i.e., chlorpyrifos) exposure. Yellow represents properties of the organisms being modeled, in particular, the life-history stages and transitions between them, behaviors (such as movement or avoidance), and energetics (if energetics of the modeled population are represented explicitly, e.g., with a dynamic energy budget). The organism-level properties being modeled are shown in more detail in the box-and-arrow diagram in the center of the CMD. The aster model (Figure 6a) includes life-history stages and transitions between them (e.g., seedlings growing in size or transitioning to rosettes). There is no behavior or energetics, and hence those features are grayed out in the left panel of the CMD. Likewise, the fathead minnow model (Figure 6b) contains a simple representation of life-history stages and their transitions, but no other organism-level properties. Other features of the model (which may refer to the environment or the individuals being simulated or both) are depicted in orange. In the aster model, density dependence, resulting from intra- and interspecific competition for light, stochasticity in the spatial location of plants, and spatial heterogeneity in pesticide exposure are included as other features (Figure 6a), whereas the simpler fathead minnow model includes no additional features (Figure 6b).

The text boxes on the top of Figures 5 and 6 show more detail on which drivers and other model features are included in the model in colors corresponding to those same features in the left panel. The diagram in the center of Figures 5 and 6 shows the modeled life stages (rectangles), the transitions between them (arrows, with or without text descriptors), and other organism-level features if relevant (ovals). Those life stages or transitions that are potentially impacted by chemicals (e.g., responses for which toxicity test data are available) are shown in red text. Any features of the organisms or the environment that include stochasticity are shown in italics; those features affected by density dependence are underlined; features impacted by spatial heterogeneity are outlined in orange. For example, in the template for Figure 5, the organisms have four life stages (egg, juvenile, subadult, and adult). The diagram shows transitions from one life stage to the next by growth/development or reproduction (arrows connecting rectangles) as well as the survival of each life stage (curved arrows below each rectangle). In this example, survival of all the life stages is a stochastic process (life stage names shown in italics). The model includes an energetics submodel for all life stages, and the adult life stage undergoes migration (shown by ovals connected to the relevant life stages). Migration is a density-dependent process (shown by underlined text), and the chemical driver is assumed to affect juvenile growth and development (shown by red text for this life stage). Because the chemical exposure is assumed to be spatially heterogeneous, the juvenile life stage exposed to the chemical is outlined in orange.

Generic model outputs are depicted in blue on the left side of the CMD with more specific details shown to the right. These are generally characteristics of population-level dynamics (such as population growth rate or population size over time) but may also include individual-level outputs (e.g., nesting success), as needed for the specific ERA for populations exposed to certain (chemical) stressors. For example, in the aster model, the main model outputs are total and flowering plant density, stage structure, and years to quasi-extinction (Figure 6a), whereas in the fathead minnow model, the main model outputs are population abundance and life-stage distribution (Figure 6b).

Preliminary tests of the standardized format by the authors using our own models revealed two important limitations. We found that creating the standard CMDs "by hand", using software such as Powerpoint or other professional graphics software (e.g., Adobe Illustrator, Inkscape), was both more time-consuming than desirable and resulted in CMDs that were more variable among users than we had hoped. In order to resolve these issues, we created a free web app ("POP-CMD-APP"pop-cmd.com) that automatically generates a diagram based on user input. The process of auto-generating diagrams ensures that the overall appearance and thus readability of the diagrams remains standardized from model to model. The left-hand text boxes of key elements include dropdown menus in which the user can quickly select, insert, or edit specific details for their model, which the POP-CMD-APP then automatically renders as visual components in the diagram.

The POP-CMD-APP user can also add specific labels to the arrows in the diagram to describe how the elements relate to each other. This is done in the aster model but not the fathead minnow model (compare Figures 6a and 6b). We anticipate that population modelers can use the POP-CMD-APP to generate diagrams for use in publications, presentations, as part of the developmental process, or in any other circumstance in which the modeler needs to quickly and easily communicate the salient features of their model. Overall, we aim to make POP-CMD-APP diagrams easily interpretable to both modelers and non-modelers alike. A user manual for the POP-CMD-APP is available at pop-cmd.com (Crouse et al. 2023), and the underlying code has been published on GitHub. Whether or not users employ the POP-CMD-APP or draw their CMDs using other software, we recommend that the features described above be followed as closely as possible to maximize consistency. The more complexity that is included in a model, the more challenging for the modeler to decide how much detail to include in this high-level visual overview. It may not be feasible to capture all of the complexities in the CMD, and some may need to be relegated to the text description, i.e., the Details portion of the ODD.

CONCLUSIONS

Population models are becoming increasingly important tools for ERA. Ensuring that sufficient guidance and standardization are available on all aspects of the modeling process should help to increase their acceptance by decision makers. Consistent model documentation following the Overview, Design concepts, and Details (ODD) protocol of Grimm et al. (2006, 2010; 2020), clearly articulated decision steps following Pop-GUIDE, and standardized conceptual models (verbal and diagrammatic) can improve model transparency and consistency. However, standardizing conceptual model diagrams (CMDs) to improve communication among modelers and between modelers and other stakeholders has not been fully addressed thus far. Here we provide the first guidance on how a CMD should be built and a tool to make this process easy and consistent. While more complex and model-specific diagrams may still be created by modelers when deemed necessary, we suggest always adding the standardized CMD presented in this paper. A good CMD can serve as an Executive Summary of the model and is a helpful tool for communicating it to different audiences. To be able to monitor the use of the standardized CMD template and thereby be able to improve it and its use, this article should be cited whenever the template is used. For ODD, this monitoring based on citations was essential to improve ODD itself and its use (Grimm et al. 2020).

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CRediT Author Statement

Valery Forbes: Conceptualization, software development, visualization, writing original draft, review, editing; **Chiara Accolla**: Visualization, writing original draft, review, editing; **Thomas Banitz:** Visualization, writing original draft, review, editing; **Kristin Crouse:** Software development, visualization, writing original draft, review, editing; **Nika Galic**: Visualization, writing original draft, review, editing; **Volker Grimm:** Visualization, writing original draft, review, editing; **Sandy Raimondo**: Visualization, writing original draft, review, editing; **Amelie Schmolke:** Visualization, writing original draft, review, editing; **Maxime Vaugeois:** Visualization, writing original draft, review, editing;

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Figure Captions

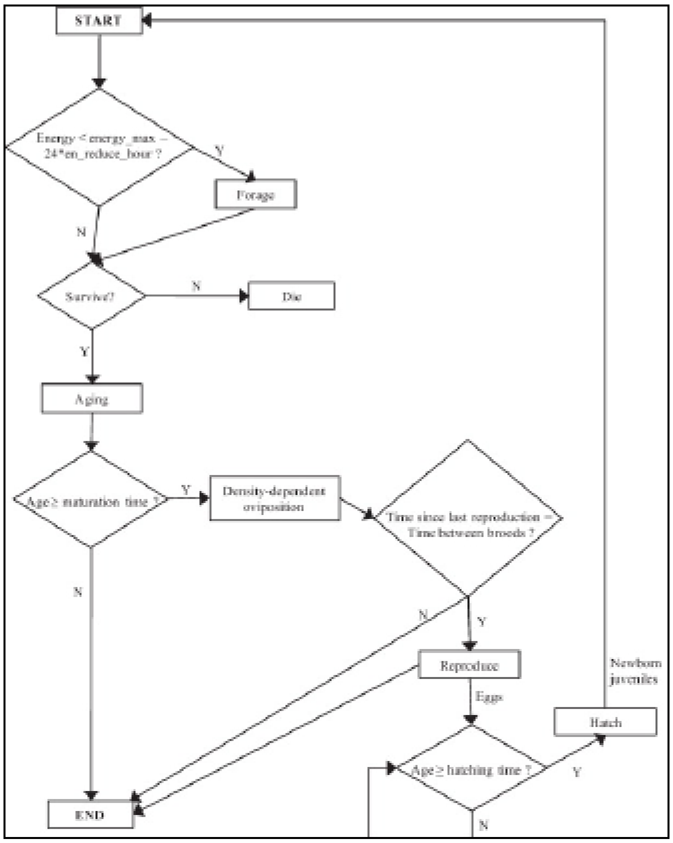

Figure 1. Conceptual model diagram (called a flow chart) from Meli et al. (2013) for an agent-based population model of the collembolan, *Folsomia candida*, that was used to explore the potential consequences of spatially heterogeneous exposure to heavy metals on population dynamics. The diagram shows the processes executed by individuals in the model. Republished with permission.

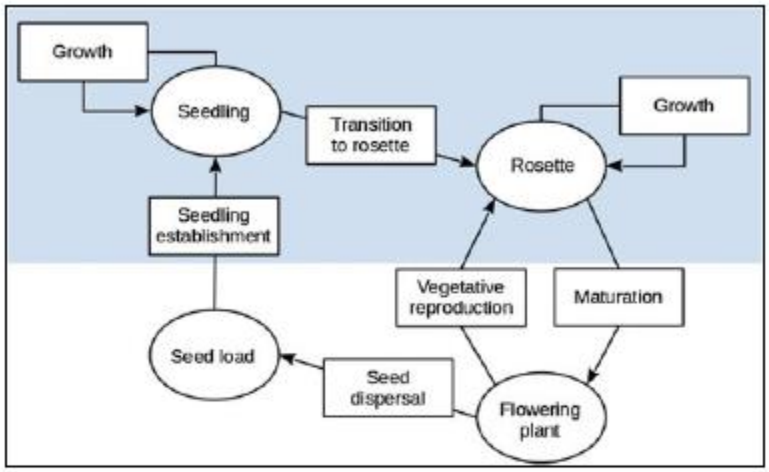

Figure 2. Conceptual model diagram (called a flow chart) from Schmolke et al. (2017) for an agent-based population model of the threatened terrestrial plant, *Boltonia decurrens*, that was used to explore the potential consequences of pesticide exposure, intra- and inter-specific competition, and flooding, on population dynamics. The diagram shows the main model processes (rectangles) and life stages (ellipses). Republished with permission.

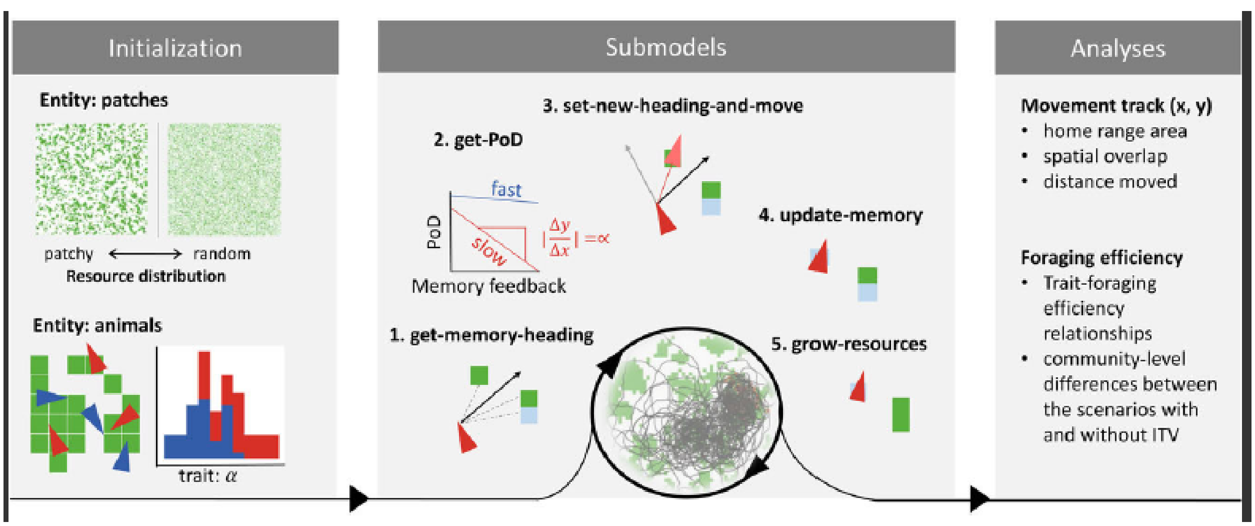

Figure 3. Conceptual model diagram (called a visual ODD) from Milles et al. (2020)) for an agent-based model designed to explore how intraspecific variation in personality-related movement behavior promotes coexistence. The figure provides an overview of the

entities and how they are initialized, the processes and their scheduling, and the key model output (observation). Republished with permission.

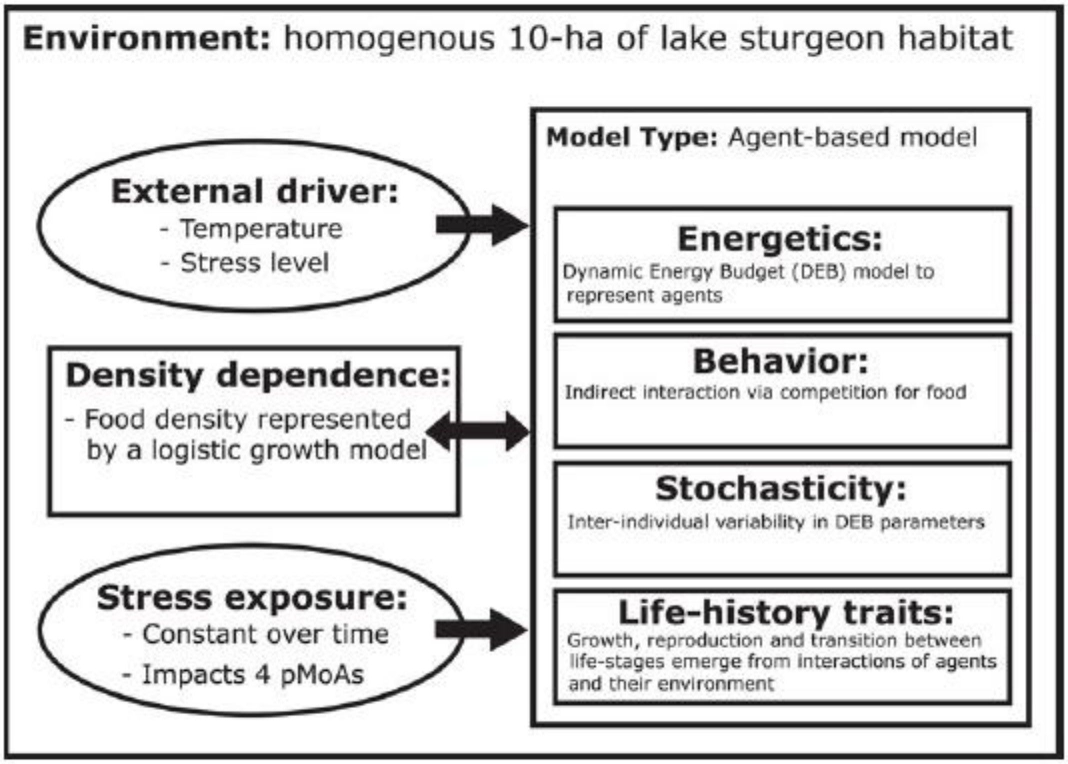

Figure 4. Conceptual model diagram from Vaugeois et al. (2022) for an agent-based model of lake sturgeon based on Dynamic Energy Budget theory to explore how contaminants of emerging concern may impact sturgeon populations. Republished with permission.

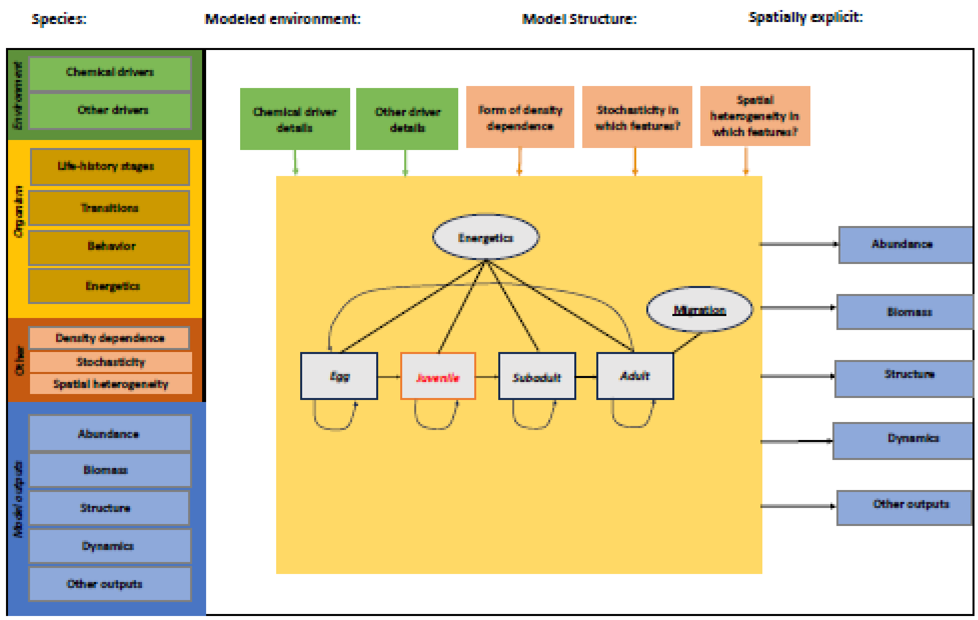

Figure 5. Standard template for a conceptual model diagram. Boxes along the left refer to key features to consider for inclusion; those not included will be grayed out. Green boxes represent aspects of the environment, particularly any external drivers (including chemicals) that may influence population dynamics. Yellow boxes represent properties of the organisms being modeled, in particular, the life-history stages and transitions between them, behaviors (such as movement or avoidance), and energetics. These are shown in more detail in the box and arrow diagram in the center of the CMD. Orange boxes represent other features of the model (which may refer to the environment or the individuals being simulated or both). Boxes at the top provide more detail on the included key features. Blue boxes along the right provide detail on the model outputs.

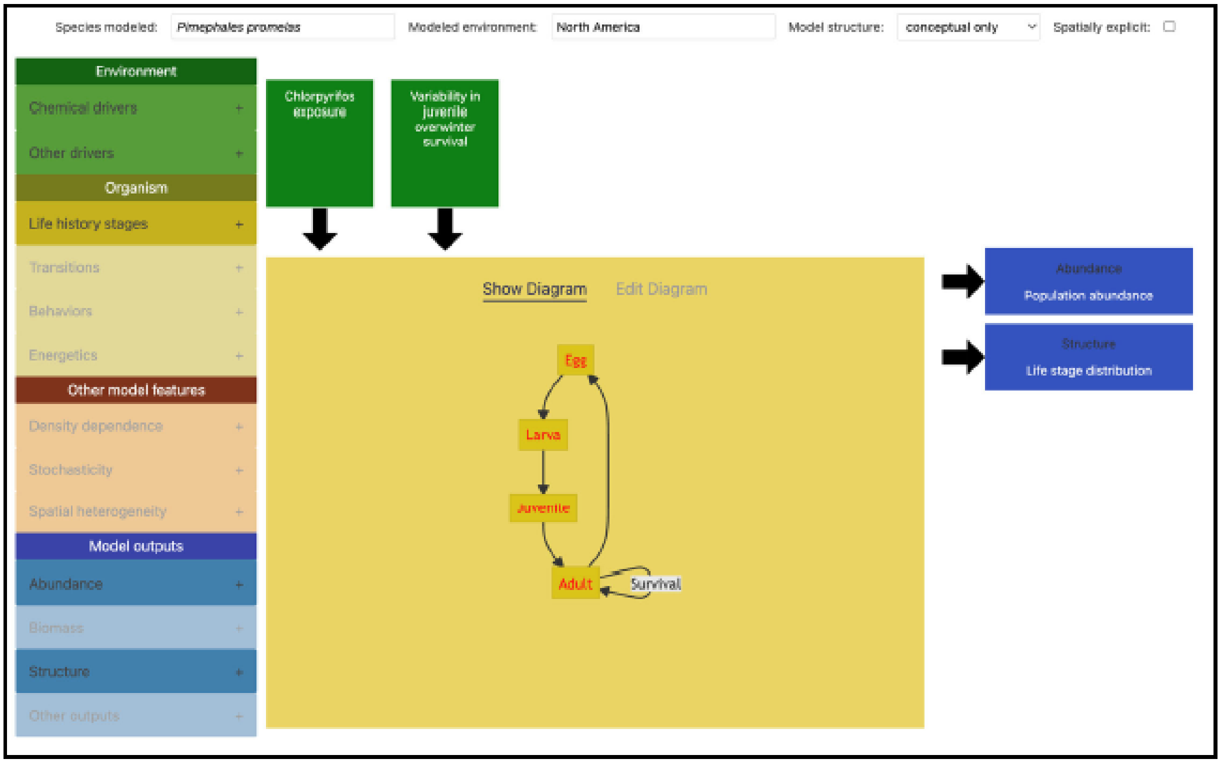

Figure 6. Conceptual model diagrams created with the POP-CMD-APP (pop-cmd.com).

A) The top figure shows a conceptual model diagram for the decurrent false aster, *Boltonia decurrens*, population model from Schmolke et al. (2017). B) The bottom figure shows a conceptual model diagram for the fathead minnow, *Pimephales promelas*, population model from Raimondo et al. (2021). See text for details.

Table 1. Types of elements typically included in conceptual model diagrams and their definitions.

Element	Definition
State variables	Set of variables used to describe the state of the dynamical system of interest (e.g., size, age, location of a population, subpopulations or classes, or individuals; living and non-living components of the environment)
Processes	Life-history events (e.g., birth, death, reproduction), behaviors (e.g., movement, mating behavior, feeding), biotic-abiotic

	interactions (e.g., uptake of resources, chemicals), abiotic processes (e.g., transport or conversion of chemicals). Some of these processes may depend on population density.
External drivers	Factors external to the modeled dynamical system of interest (e.g., flood, fire, temperature, chemicals), but inherent properties of nature that influence processes; can be called parameters when constant and forcing variables when not
Stochasticity	Random variability in processes, external drivers, or initial system states
Spatial heterogeneity	Some elements of a model may vary spatially (e.g., exposure to chemicals). Models that are spatially explicit incorporate this heterogeneity, often by simulating the modeled environment as a series of grids.
Outputs	System characteristics that the model generates (population size, structure, biomass, etc.) and on which the risk assessment can be based; often these are at the population level but may also include individual-level characteristics (e.g., nest success, home range, etc.)