QUESTIONS FOR MODELING STUDY DESIGN

COMMUNITY OF PRACTICE FOR STATISTICS
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Model development is a naturally iterative process, i.e. results from early model development activities frequently inform and enhance later modeling efforts. This may lead to methodology changes or refinements that improve model performance and enhance fitness for purpose.

Model Purpose

- Has sufficient detail been provided to explain why a model is needed and to define its intended application?
- Does the explanation distinguish between developing a new model and modifying an existing model for a different purpose?
- Is the intended application clearly defined, including the intended scope of the model's application and its known limitations?

Model Structure

- Is the model's structure consistent with the stated model purpose?
- Are the model's objectives and assumptions defined?
- Is the type and scope of model to be developed clearly defined and presented, including a diagram or flow chart if applicable?
- Are the criteria or rationale for the model structure provided?

Mathematical Representation

- Are the equations used in the model explicitly described? Or, for larger models, is a complete set of generic equations provided and described?
- Do the equations' descriptions include text that describes what the mathematics represents?
- Are all units of parameters identified?

Input Data Requirements

- Are the model inputs defined by type and source?
- Are the model inputs characterized in terms of necessary quality criteria appropriate to its application?

Parameter Estimation

- Are all parameters listed and defined, with data sources referenced?
- Are parameter estimation methods (calibration) described?
- Are quality objectives and acceptance criteria included?

Computer Implementation

- Are computer hardware and software requirements identified, including any requirements for model code development?

- Are steps in place to verify either proper implementation of existing software algorithms or proper development of new code?

Evaluation of Predictive Capacity

- Are the datasets needed for model evaluation (e.g., experimental or field observations) identified, as well as what model endpoints or outputs will be assessed?
- Are the methods (e.g., metrics, graphical-based summaries, statistical models, etc.) for evaluating the model's predictions identified?
- Are the model endpoints that will be evaluated consistent with the model endpoints that will be used to answer the research questions of interest?
- Are the criteria for judging whether the model's performance is adequate for its designated task identified?

Sensitivity and Uncertainty Analysis

- Are the model inputs, parameters, or options that will be included in the sensitivity and/or uncertainty analysis identified?
- How will the sensitivity and/or uncertainty analysis be used to communicate the level of confidence in model-predicted values in a way that is easy for model users and decision-makers to interpret?

GUIDANCE FOR REVIEWING
PROJECT PROPOSALS FOR MODELING

Preface

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Outline of Coverage

Model Purpose
Model Structure
Mathematical Representation
Input Data Requirements
Parameter Estimation
Computer Implementation
Evaluation of Predictive Capacity
Sensitivity and Uncertainty Analyses

Model Purpose

The purpose or application for which a physiological or environmental model is developed guides and informs its structure, model inputs (parameterization), level of detail and type/extent of model evaluation required. For example, a model originally developed for a specific research use (e.g., experimental design, hypothesis testing) may not be applicable to or meet the necessary criteria for application in regulatory decision making without significant modification (U.S. Environmental Protection Agency [USEPA] 2006). Thus, research planning documents need to describe the intended application of a newly developed or modified model in sufficient detail to allow determination of whether a particular model is likely to be "fit for purpose" at the conclusion of the project. The statement of purpose needs to provide adequate background information to facilitate understanding why a model is necessary and to define the conditions under which the model is intended to be used, as well as any known limitations of the model. This is sometimes referred to as defining the scope or domain of model applicability.

Model Structure

The structure of any model largely depends on the purpose for which the model is being developed. There is virtually no limit to the complexity of a model's construction, but the description of the relationships among the variables and processes being integrated needs to be thorough enough to provide reproducible results.

Model development involves a collaborative and iterative process to identify all the components that must be factored into the design to address the defined purpose. Consideration must be given to defining the objectives, determining the type and scope of model required, determining the data criteria, defining the model's applicability and identifying any constraints. Once the answers to these questions have been determined, the framework can be selected for defining the model structure for development.

Mathematical Representation

After the purpose and structure of the model have been identified, the mathematical equations that represent the qualitative structure of the model must be specified. The differential and algebraic equations of the model should be provided in sufficient detail to allow an independent investigator to use them to develop a functional version of the model. Specifications for smaller models should explicitly provide all the equations of the model; for larger models, a set of generic equations can be provided. The units of measurement for each parameter should be indicated, as well as the overall unit of each equation. Each equation should be accompanied by text that explains exactly what the mathematics represents. Finally, the equations should be drawn using the equation editor in Microsoft Word or an equivalent package.

Input Data Requirements

Research planning documents should include definitions of model inputs, their sources, and any relevant quality criteria. Model inputs are numerical values (parameters) describing chemical, biological or environmental variables that are incorporated into the model to allow simulation or prediction of the environmental or biological outputs of interest. These variables may be described either as point estimates or as ranges of values, depending upon the modeling application. Input data requirements are defined by the purpose of the model and its intended domain of applicability. Types of model inputs, their sources, and any information necessary to evaluate their quality, variability and uncertainty can be important determinants of the reliability of model predictions.

Parameter Estimation

The U.S. Environmental Protection Agency (EPA) defines a model's parameters as "terms in the model that are fixed during a model run or simulation but can be changed in different runs, either to conduct sensitivity analysis or to perform an uncertainty analysis when probabilistic distributions are selected to model parameters or achieve calibration goals" (USEPA 2009). Parameters can be constants, such as the speed of light, or quantities estimated from sample data that characterize statistical populations, such as a population growth rate. Quality assurance of model parameters is important for overall model quality.

Parameter estimation, or model calibration, is the process of adjusting parameters within physically defensible ranges to refine the model to achieve a desired degree of correspondence between the model's output and actual observations of the environmental system the model is intended to represent (USEPA 2002). EPA recommends that the following elements be documented when estimating parameters: the data used for parameter estimation, the rationale for estimates in the absence of data, and the reliability of parameter estimates. The quality assurance plan should include objectives that guide the modeling process and specify goals for calibration. Modelers should also provide acceptance criteria**:** the specific limits, standards, goodness-of-fit, or other criteria on which a model will be judged as being properly calibrated (USEPA 2009).

Computer Implementation

Most models require the use of numerical simulation methods, including solutions of differential equations or optimization routines (USEPA 2006). Computer implementation of models includes identifying algorithms to use, identifying hardware and software requirements, specifying inputs, implementing computational methods, and documenting the results (USEPA 2009). If a tool is being developed, computer implementation also may include developing a user interface and operating instructions.

Many commercially available software packages are available to implement algorithms to obtain mathematical solutions, so that the modeler only needs to determine that an appropriate algorithm is used and that it is implemented correctly. If a programming language (e.g., C++, Fortran, R) or spreadsheet functions (e.g., Microsoft Excel) are used, the modeler should write code—and document its development—for an appropriate algorithm, including frequent debugging or diagnostic checks to detect syntax errors, verify model output and ensure correct mathematical representation of a process. Several techniques can help minimize programming errors and facilitate code verification, including using comment lines to describe components of the code, using a flow chart to describe the structure of the model program, breaking large programs into discrete modules and using generic algorithms, packages or publicly available "recipes" for common tasks (USEPA 2009).

Evaluation of Predictive Capacity

The purpose of model evaluation is to assess the adequacy of a model to describe the system of interest, as well as the suitability and applicability of the model for the regulatory-, health- or ecological-related application of interest. Evaluation methods and metrics for validation of model output depend on the context in which the models are to be applied. It is usually the case that no single approach will be sufficient for a thorough evaluation of model predictions, but a variety of methods (e.g. graphical, cross-validation, comparison of statistical metrics to available "benchmarks," analysis of residuals, etc.) will need to be employed. Before model development begins, an evaluation plan should be in place that describes what datasets will be used to compare to model output and that clearly explains how the evaluation results will be suitable for judging whether or not the model's performance is adequate for the intended application. The evaluation results should guide model improvement and direct resources to areas needed for additional data collection.

Sensitivity and Uncertainty Analysis

Frequently, certain aspects of a modeling system are inherently more uncertain than others due to differences in the underlying inputs or scientific understanding that is used to develop the various parts of the system. Therefore, the impact of these data gaps on the decision making process should be transparent and clearly communicated. Sensitivity and uncertainty analysis can thus be an important step in establishing the credibility of model predictions and identifying what improvements to model processes or inputs will most reduce the uncertainty in the final predicted value.

Sensitivity analysis evaluates the effect of changes in model inputs or assumptions on a model's results (USEPA 2009). Sensitivity studies are often used to focus resources for more detailed analysis and identify what improvements are needed to reduce the model's uncertainty (USEPA 2006). For example, a sensitivity analysis can be used to identify what model inputs, parameters or specifications are of greatest interest in a supplemental uncertainty analysis. There may be a large degree of uncertainty in the specification of a particular model input or parameter, but if the model endpoint of interest is found to be insensitive to large changes in this model element, then additional quantification of model uncertainty is not needed.

Uncertainty analysis quantifies the lack of knowledge and other potential sources of error in various components of the modeling systems, and it investigates the effect this uncertainty has on model outputs (USEPA 2009). Uncertainty analysis provides quantitative information on the confidence the model user should have in the model output. Such an analysis also can be used to establish what, among various sources of uncertainty, contributes most to the uncertainty in the final model prediction. For example if a model's predictions were found to be highly uncertain but the major source of uncertainty was due to uncertainty in a particular input, then resources should be directed toward improving the model inputs, rather than toward refining the model specification itself (Beck et al. 1997).

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Additional Resources

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