



Standard Practice for Evaluating Mathematical Models for the Environmental Fate of Chemicals¹

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1. Scope

1.1 This practice provides procedures and criteria for development, modification, and use of mathematical models to integrate knowledge of environmental partitioning, transport, and transformation for use in predictive risk assessments. The exposure assessments may subsequently be used in chronic or acute health risk assessments. It does not specify models themselves, but it establishes minimum criteria for distinguishing acceptable models from those that may be incomplete, untested, or inappropriate for intended uses.

1.2 The practice is applicable to models within and among environmental media (air, water, solids, and biota) and it addresses evaluation of the generic characteristics of all such models.

2. Referenced Documents

2.1 ASTM Standards:

E 943 Terminology Relating to Biological Effects and Environmental Fate²

2.2 National Technical Information Service:³
Chemical and Biological Abstracts

3. Terminology

3.1 Definition:

3.1.1 *environmental fate*—describes the form and location of a material resulting from many processes, including transport, environmental partitioning, and transformation. (See Terminology E 943.)

3.2 Description of Terms Specific to This Standard:

3.2.1 *algorithm*—the numerical technique embodied in the computer code that defines a set of rules to solve the governing equations in a finite number of steps. The governing equations represent a mathematical description of the system, and may include a transformation process, a transport process, chemical partitioning, physical property variation with temperature, etc.

3.2.2 *calibration*—a test of a model with known input and

output information that is used to adjust or estimate coefficient or parameter values.

3.2.3 *compartmentalization*—division of the environment into discrete intervals in time, space or environmental media.

3.2.4 *computer code (computer program)*—the assemblage of statements written in a programming language that accept input data, solve the governing mathematical equations using the specified algorithm, and provide output information.

3.2.5 *model*—an assemblage of concepts in the form of equations that represent a mathematical interpretation of a natural phenomenon.

3.2.6 *sensitivity*—the degree to which the model result is affected by changes in a selected input parameter. It is often defined as the ratio of the percent change in the model result divided by the percent change in the selected input parameter (1).⁴

3.2.7 *validation*—a test of the model with known input and output information that is used to assess that the calibration parameters are accurate without further change. Preferably, it should represent a different physiochemical condition than used for model calibration.

3.2.8 *verification*—examination of the numerical technique in the computer code to ascertain that it truly represents the conceptual model and that there are no inherent numerical problems with obtaining a solution.

4. Significance and Use

4.1 This practice permits the orderly evaluation of models for their completeness and suitability in specified uses. Numerous mathematical models have been and are being developed for use in estimating the movement and distribution of natural and anthropogenic chemicals in the environment as part of exposure assessments. Such assessments predict whether human activities might result in violation of policies set forth by the National Environmental Policy Act (NEPA) of 1969 and the various requirements of the Environmental Protection Agency (EPA), the Nuclear Regulatory Commission (NRC), and other federal and state agencies. The ultimate objective of these models is to predict the concentrations of chemicals to which organisms, including man, may be exposed following short or long-term releases of the chemical to the environment.

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² Annual Book of ASTM Standards, Vol 11.05.

³ Available from National Technical Information Service, Springfield, VA 22151.

⁴ The boldface numbers in parentheses refer to the list of references at the end of this practice.

Due to differences in intended uses, the models range in complexity from simple algebraic expressions suitable for hand calculation, to multiple differential equations linked to environmental data in ways that require the calculation power, bookkeeping routines, and data storage capabilities of computers.

4.2 Numerous pressures have led to the application of these models in varying stages of completion, documentation, public availability, testing, and evaluation. Often these models are used without any foreknowledge of the confidence that can be placed in their predictive capabilities. Different models intended for similar uses incorporate special features (for example, temporal and spatial definitions and units) that make intercomparisons difficult. Models can be used in ways that violate the assumptions and boundary conditions that are built into them. Such deficiencies and differences in extant models have led to unnecessary conflicts among users. This practice outlines evaluation procedures and criteria that may be followed by model developers in bringing their models to a level of general acceptability, and may be used by model users as a standard yardstick to evaluate models and their appropriate uses (that is, prevent use outside the limits of the assumptions used to formulate the model).

4.3 When selecting a model for use, it is important to understand its purpose. A model selected for range finding could be quite different from one selected for quantitative predication. In general, we might consider four modeling purposes, each with an expected degree of acceptable accuracy.

Modeling Purpose	Acceptable Accuracy	Model Class
Range Finding	Order of magnitude	1
Screening	Multiple of 2 or 3	2
Classifying	±35 to 50 %	3
Predictive	±5 to 15 %	4

4.3.1 Each situation has a unique set of conditions that define acceptable accuracy and it is the responsibility of the individual modeler to define what is acceptable. For example, acceptable accuracy for a regional groundwater model (scale of kilometres) is generally less rigid than for a local model (perhaps a scale of tens of metres). As will be discussed later, it is also the responsibility of the modeler to ensure that model selection is appropriate for the model purpose. Simple models are generally appropriate for qualitative assessments, such as range finding and screening, whereas it may be necessary to use a much more complex model to achieve the acceptable accuracy necessary for predictive simulations.

4.4 This practice is not meant to standardize models themselves (in concept, level of complexity, or uses) or to select any specific model(s) or ASTM approval or sanction.

5. Model Classification

5.1 The manner in which models are evaluated will depend on the kinds of models being examined and the purpose of the modeling to be performed. Sensitivity and validation studies, for example, require different handling of the input data for different model types. The equations used to model environmental processes should reflect the best mathematical approach available to represent that process including equilibrium partitioning, steady state modeling, and kinetics of dynamic solutions for the equations selected. Three different kinds of

exposure assessment models are in common use (2). These are the multiplicative chain models (MCMs), linear systems models and complex models. In addition, analytical models could be added.

5.2 *Multiplicative Chain Models* use mathematical relationships of the form:

$$z = A \frac{x_1 x_2 \cdots x_m}{y_1 y_2 \cdots y_n} \quad (1)$$

where:

- z = concentration of material or a measure of impact on health (such as dose),
- A = a constant, and
- $x_1 \cdots x_m, y_1 \cdots y_n$ = measurable environmental quantities such as concentration.

The ratio x_1/y_1 might be a bioaccumulation factor or a concentration ratio (3).

5.2.1 Multiplicative chain models are frequently used to estimate the transport of materials through terrestrial and aquatic environments. The computer code SARAH2 is an example (4, 5).

5.3 *Linear-Systems Models* are characterized by a system of first-order, linear, coupled differential equations that describe rate of transfer of mass or energy from one environmental compartment to another. The coefficients in the differential equations represent transfer rates that can be assumed to obey zero or first-order relationships. The solution of a linear-systems model describes the content (or concentration) of a chemical in a given compartment as a function of time. An example of a linear-systems model that describes the bioaccumulation of nonpolar organic chemicals by fish from both water and tainted food is the computer code FGETS (5, 6, 7).

5.4 *Analytical Models* are characterized by closed-form, or *analytic*, solutions to the governing equations. Multiplicative chain models and some linear-system models are analytic in form. However, under certain assumptions, high order equations can have analytic solutions (for example, advection-dispersion under steady uniform flow with constant coefficients).

5.5 *Complex Models* do not fall into any of the other three categories. These may be characterized (although not necessarily) as nonlinear models, distributed system parameter models (8), or models for which there exists no tractable analytic solution relating the inputs to the outputs. In these cases, a numerical solution algorithm is used to solve the governing equations in approximate form on a computer. An example is the computer code CE-QUAL-W2 (9).

5.6 *Model Classification* can be used to differentiate between various model types. Most topical areas, including the fate of materials in the environment, can be viewed as having a hierarchy of differing levels of spatial and temporal resolution. Generally, simple models have few compartments and may be steady state, whereas complex models may have detailed resolution and be dynamic. Ambrose et al (10) proposed the following four levels of sophistication that proved useful for evaluating water quality models:

5.6.1 *Level 1*—Simple manual, graphical, or analytical techniques, that can be useful as a crude screening methodology.

These may include ideal and nonideal equilibrium partitioning models.

5.6.2 *Level 2*—Simple computerized techniques, that can be useful as a fine screening, or for crude planning and assessments. These techniques include steady-state models that allow spatial variability in geometry and environmental parameters.

5.6.3 *Level 3*—Intermediate computerized techniques, that can be useful for fine planning, or crude engineering and management design. These techniques include steady-state flow models with dynamic water quality processes, and dynamic, one-dimensional branching models.

5.6.4 *Level 4*—Advanced computerized techniques, that can be used for detailed engineering design and management plans. These techniques include dynamic, multidimensional models.

5.7 *Steady State and Dynamic Models* are alternative classifications that are related to the levels of compartmentalization described in 5.6. When only one or a few compartments are included in a model (Levels 1 or 2), it may be possible to characterize the important model inputs as time invariant and simple steady-state models or time variable models with analytical solutions may be used. As the degree of compartmentalization is increased, the number of model parameters to be characterized as time invariant becomes untenable, and this practical simplification (that is, steady state) is no longer justified. Thus the difficulty of solving the underlying system of equations becomes increasingly complex. Analytical solutions become increasingly difficult to obtain and more computationally intensive numerical methods are required. Hence it may be necessary to use a more dynamic type of simulation model (Levels 3 or 4).

5.7.1 In addition to the degree of compartmentalization of the model, the environmental setting can also control the type of model that is used. Environmental contaminants of interest are frequently associated with time constants that are on the order of weeks to months and are therefore exposed to wide variations of environmental conditions (for example, rainfall, runoff/stream flow, temperature). Simple Level 1 models may still be useful, however, for performing screening level calculations, even when steady-state conditions are not strictly applicable. For example, the use of worst-case assumptions as part of the steady-state analysis may be overly conservative, but still adequate to demonstrate that adverse levels of a contaminant will not occur. For example, knowing that the instream level of a pesticide applied to a field would not exceed a critical stream standard even if it were all added at one time to the stream during a critical low flow condition, would preclude the need for using a complex agricultural runoff and receiving water model. When the results are not definitive from this type of analysis (that is, the critical concentration would be exceeded under the worst-case assumptions), more detailed investigations using increasingly complex models (Levels 2, 3, or 4) may be warranted. For this reason the more complex dynamic models are frequently used, especially when a relatively high degree of precision is required. The lower level of effort and cost associated with the simpler models, and the insight that may be gained from their use, may still justify their application however, even when more complex methods are subsequently used.

6. Model Evaluation

6.1 *Program Examination* determines whether the concepts in a model adequately represent the phenomena, processes and actions that are of interest to model users. This determination involves answering such questions as: Are the relevant physical, chemical, biological and toxicological phenomena properly included in the equations? Are the equations representing the various state variables valid within the intended range of applicability of the model? Are the equations mathematically well-behaved within the intended range of model applicability? Are the boundary conditions and initial conditions appropriate? Is the approach to the solution the most appropriate one for the intended model application? Is the range of applicability adequately defined and appropriate? Has the model's performance been demonstrated or field validated as an accurate representation of the processes being modeled?

6.1.1 If the program being examined is judged to adequately represent the phenomena of interest for the purposes intended, the program can then be designated for inclusion within a program inventory. If deficiencies are found and deemed serious, the program should not be used for exposure assessments. A recommendation might be made to submit the program to major conceptual and programming modifications if no suitable alternate program is available.

6.2 *Model Evaluation*, consists of seven major tasks. A useful approach to program selection and model development that can be generically applied is found in Walton et al (11).

6.2.1 *Model Conceptualization*, involves determining the important processes that must be included in the model description, and their linkage, to be able to adequately represent the system being studied.

6.2.2 *Program Examination*, involves questioning whether anything fundamental was omitted in the initial model conceptualization.

6.2.3 *Algorithm Examination*, evaluates whether appropriate numerical schemes have been adopted to represent the model in the form of a computer code. Factors to be considered include accuracy, convergence, stability, efficiency and reliability.

6.2.4 *Data Evaluation*, is intended to ascertain the quality and the quantity of the input and output data available for use with the model.

6.2.5 *Sensitivity Analyses*, are studies directed toward identifying those parameters that are most influential in determining model predictions. In general, if the conclusion drawn from the model application would change, based on varying parameters over estimated or statistical ranges, then more information (data) must be provided. The identification of key parameters enables priorities to be established for gathering additional data, including performing experiments. Approaches are described in 6.5.

6.2.6 *Validation*, refers to simulations to determine the degree to which model predictions agree with field or laboratory measurements of those same quantities, without altering model coefficients following calibration.

6.2.7 *Code Comparison*, is the process of comparing the strengths and weaknesses of various codes designed to perform similar tasks. Often there is more than one model or computer