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Project Summary

Guidelines for Field Testing Aquatic Fate and Transport Models: Final Report

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These guidelines have been written for the Office of Pesticides and Toxic Substances (OPTS) U.S. EPA as an aid in field validation of aquatic fate and transport models. Included are discussions of the major steps in validating models and sections on the individual fate and transport processes: biotransformation, oxidation, hydrolysis, photolysis, ionization, sorption, bioconcentration, volatilization, and physical transport. For each process, the following information is provided: a general description of the process, a list and discussion of environmental factors affecting the process, a list of the priority pollutants for which the process is important, a list of model-specific environmental inputs, and field methods for collecting these input data.

This Project Summary was developed by EPA's Environmental Monitoring Systems Laboratory, Las Vegas, NV, to announce key findings of the research project that is fully documented in a separate report of the same title (see Project Report ordering information at back).

Introduction

Aquatic fate and transport models have been developed which predict the fate and concentration of chemicals released into natural waters. These models may be based upon either an empirical approach or a theoretical approach that considers transport and fate processes. Empirical models, which are based on extensive field observation, are usually calibrated to specific existing sites and chemicals and provide no rational basis for making predictions outside their range of prior observation. Thus, models of this type are generally not suited to predicting the fate of new chemicals and are not considered in these guidelines.

The theoretical approach is based upon an understanding of environmental fate and transport processes, including biotransformation, hydrolysis, oxidation, photolysis, ionization, sorption, volatilization, bioconcentration and physical transport. This type of model is considerably more versatile, since it is designed to predict environmental fate and pollutant concentrations based upon degradation rate constants and relatively simple chemical and environmental input data. Therefore, theoretical models can be applied to chemicals which have not yet been introduced into the environment. Such models are of considerable interest to the U.S. EPA and, in particular, the OPTS.

Guidelines

The guidance provided consists of a beginning section which addresses the steps in validation. Subsequent sections cover the environmental fate processes and field methods for collecting environmental input and output data. The major steps in the field validation process are outlined in Table 1.

Validation of a model is defined in this report as a comparison of model results with numerical data derived from observations of the environment. Complete model validation requires testing over the full range of conditions for which predictions are intended. At a minimum, this requires a series of validations in various aquatic environments (streams, lakes, estuaries) with chemicals that typify the major fate and transport process. Vali-

Table 1. *Steps in Field Validation of Aquatic Fate and Transport Models*

Step 1.	*Identify Model User's Needs: The first step in field validation is to obtain a clear understanding of the model user's needs and how the model would be used.*
Step 2.	*Develop Acceptance Criteria for validations: The potential model user should provide criteria against which the model is to be judged.*
Step 3.	*Examine the Model: This step involves a detailed examination of the model to precisely define input data requirements, output predictions and model assumptions.*
Step 4.	*Evaluate the Feasibility of Field Validation: It may not be feasible to attempt field validation for some models, and the validator should consider this possibility.*
Step 5.	*Determine Validation Scenario: There are many different approaches to field validation and a scenario should be identified or approved by the potential model user.*
Step 6.	*Plan and Conduct field validations by performing the following steps:*
Step 6a.	*Select a Site and Compound(s): There are many factors to consider in selecting a site and compound(s).*
Step 6b.	*Collect Preliminary Data and conduct Sensitivity Analyses: Preliminary data are required to conduct a sensitivity analysis and determine the most important input variables.*
Step 6c.	*Develop a Field Study Design: Development of a detailed field sampling plant for the specific model compound and site.*
Step 6d.	*Conduct Field Study: Implementation of the field plan not addressed in these guidelines.*
Step 6e.	*Analyze Samples: The document does not provide specific guidance on analytical methods and quality assurance procedures but references are provided.*
Step 6f.	*Compare Model Performance with Acceptance Criteria: Graphical and statistical comparison.*

dated models are useful in the regulatory process because they withstand scientific scrutiny and are defensible in courts of law.

Much of the information presented in the first section relates to the identification of potential problems associated with field verification of models. Where possible, solutions or approaches have been suggested, but many problems are specific to a site, compound, or model and have to be dealt with individually. An example of the type of information important in Site and Compound Selection Criteria, is depicted in Table 2.

Subsequent sections of this report deal individually with environmental fate and transport processes. For each process, the following information is given: a general description of the process, a list and discussion of environmental factors affecting the process, a list of the priority organic pollutants for which the process is important, a list of model-specific environmental inputs and, finally, field methods for collecting the model input data. Environmental inputs to several models are listed in Table 3. In addition, Table 3 includes parameters which can be important to a specific process but are not currently required model input parameters. The report also briefly covers the collection of input loading data, field sampling for predicted model outputs, and quality assurance. Experience gained during field validation of the EXAMS model was used to modify and improve this document. The guidance provided by this document was constructed for simplified aquatic fate and transport models, e.g. EXAMS. However, the steps in field validation and many of the environmental measurement techniques would apply to all aquatic fate and transport models.

Table 2. *Compound and Site Selection Criteria*

Compound Factors	
Analytical methods	*-- Methods must exist for quantifying the input loadings to the model and the concentration of the compound in environmental media.*
Compound inputs	*-- The availability of compound specific inputs such as aqueous solubility, degradation rate constants is a factor in selecting compounds.*
Environmental Fate	*-- The predicted half-life of the compound by each fate and transport process must be considered relative to the time which the compound can be followed. Ideally, the compound should be tracked through several half-lives.*
Compound Toxicity	*-- The least toxic compound representative of a given process should be selected.*
Source	*-- Select compounds that exist in concentrations that can be tracked in aquatic systems. Although many compounds have been detected in effluents, relatively few, have been found in easily detectable levels in receiving waters.*
Site Factors	
Traceable	*-- The compound of interest must be present in sufficiently high levels to be traced for considerable time or distance. Factors influencing traceability include input load, water body size, flow rate, half-life, mixing and dilution.*
Ability to collect data	*-- The collection of most site specific model input data presents no unusual problems. However, particular consideration should be given to mixing, flow sediment transport, ground water movement, weather, season, size of the water body and access.*
Historical site data	*-- If historical data are available, they can be used to conduct preliminary sensitivity analyses. Depending upon the amount and type of data, it may not be necessary to conduct a preliminary sampling study.*
Input loadings	*-- The pollutant load to the system must be known. The accuracy of these data will depend upon the types and number of sources, their relative loading, and their variability.*
Analytical problems	*-- Chemicals found in the water body to be studied may interfere with analyzing for the compound of interest. Samples or environmental media should be analyzed prior to any major field effort.*

Table 2.	*(Continued)*
Model assumptions	-- *Conditions at the site should not violate model assumptions. Proper site and compound selection offers an opportunity to design around some model assumptions.*
Type	-- *Compounds with short or long half-lives can easily be studied in small, well-mixed pounds. Rivers or streams are best suited to test the degradation or transport of short lived compounds. Long lived compounds should only be used to test physical transport and bioconcentration processes. It is usually impossible to track long lived compounds through several half-lives in rivers or streams.*
Simplicity	-- *Generally, the simpler the site in terms of the amount of data that must be obtained, the more cost effective the validation effort. Multiple sources may significantly increase expense of collecting data, increase input data and complicate data interpretation.*

Table 3. *Environmental Inputs by Process, to Aquatic Fate and Transport Models*

Biotransformation
- Temperature (C)
- Total Bacteria Pop. (Cells/ml) or (Cells/100 g dry sed.)
- Active Degrading Pop. (% of Total)
- Nutrients C/N, P (mg/l)
- Acclimation State
- PH (pH Units)
- Dissolved Oxygen (mg/l)

Hydrolysis
- POH (pH Units)
- PH (pH Units)
- Temperature (C)
- Oxidation
- Temperature (C)
- Oxidant Concentration (moles/l)
- Reaeration (cm/hr)
- Suspended Particulate (mg/l)
- Dissolved Oxygen (mg/l)
- Dissolved Organic Carbon (mg/l)

Photolysis
- Depth (m)
- Chlorophyll (mg/l)
- Latitude (degrees)
- Cloudiness (tenths)
- Dissolved Organic Carbon (mg/l)
- Suspended Sediment (mg/l)
- Spectral light intensity at surface
- Altitude (m)
- Temperature (C)
- Time of Day (24 hr time)

Ionization
- POH (pH Units)
- PH (pH Units)
- Temperature (C)
- Total Dissolved Solids (mg/l) Ionic Strength

Volatilization
- Temperature (C)
- Compartment Dimensions, area and volume
- Mixing Reaeration Rate (cm/hr)
- Wind (m/s)
- Slope (m/m)
- Water Velocity (m/s)

Sediment Sorption
- Organic Carbon Content (% of dry sediment)
- Percent Water of Benthic Sediment $\frac{(100\ \text{Fresh Wt.})}{(\ \text{Dry Wt.}\ )}$
- Bulk Density Benthic Sed. (g/cc)
- Suspended Sediment (mg/l)
- Compartment Dimensions & Areas
- Cation Exch. Cap. (meg/100 g dry sediment)
- Anion Exch. Cap. (meg/100 g dry sediment)
- Particle Size (mm)
- PH of Sediment (pH Units)

Bioconcentration
- Total Biomass (mg/l or g/m^2)
- Planktonic Biomass (fraction of total)
- Fish (g/m3)
- Water Bugs (g/m3)
- Zooplankton (g/m3)
- Phytoplankton (g/m3)
- Particulate Organic Matter (g/m3)
- Floating Particulates Organic Matter (g/m3)
- Floating Macrophytes (g/m3)
- Dissolved Organic Matter (g/m3)
- Zoobenthos (g/m^3)
- Chlorophyll a (mg/l)
- Fish by species (g/m3)
- Fish by Age or Size Class (g/m3)
- Periphyton (g/m3)
- Zoobenthos by Functional Group (g/m3)
- Temperature (C)
- Dissolved Oxygen (mg/l)
- Macrophytes, Rooted (g/m3)

Physical Transport
- Evaporation-(mm/month)
- Interflow (m3/hr)
- NPS Sediment Load (kg/hr)
- NPS Water Load (m3/hr)
- Percent Water of Bottom Sed. (100 x fresh/dry Wt. sed.)
- Rainfall (mm/month)
- Suspended Sediment (mg/l)
- Bulk Density Bottom Sed. (g/cc) Stream Inflow (m3/hr)
- Stream Borne Sediment Inflow (kg/hr)
- Compartment Volume (m3)
- Eddy Diffusivity (m2/hr) Cross Section Area for Dispersive Exchange (m2)
- Surface Area (m2) Dist. Between Compt. Centers (m)
- Compartment Dimensions L, W, H (m)
- Sediment Bed Load (kg/hr)
- Planktonic Biomass (mg/l)
- Water Velocity (m/s)
- Dissolved Organic Carbon (mg/l)
- Bed Load by Part. Size Classes (%)
- Total Organic Carbon (mg/l)

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The complete report, entitled "Guidelines for Field Testing Aquatic Fate and Transport Models: Final Report," (Order No. PB 83-222 760; Cost: $19.00, subject to change) will be available only from:

National Technical Information Service
5285 Port Royal Road
Springfield, VA 22161
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