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Project Summary

Modeling the Fate of Toxic Organic Materials in Aquatic Environments

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In the project report, documentation is given for PEST, a dynamic simulation model for evaluating the fate of toxic organic materials (TOM) in freshwater environments. PEST represents the time-varying concentration (in ppm) of given TOM in each of as many as 16 carrier compartments; it also computes the percent distribution and half life of the TOM in each of the carriers. Possible carriers include phytoplankton, macrophytes, zooplankton, waterbugs, zoobenthos, fish, particulate organic matter, floating organic matter, clay, and water (with TOM in the dissolved phase).

PEST simulates TOM degradation by hydrolysis, oxidation, photolysis, microbial metabolism, and biotransformation by higher organisms; it simulates TOM transfer by solution, volatilization, sorption, absorption onto gills, consumption, excretion, defecation, biodeposition, mortality, and throughflow. These processes are subject to time-varying environmental factors such as pH, temperature, dissolved oxygen, wind, solar radiation, and biomass and condition of organisms.

The model has been verified with process-level laboratory data and with ecosystem-level site data. The site data for fish ponds in Missouri and Israel and a reservoir in Iowa constitute prototype data sets that can be used to evaluate other compounds.

PEST is an interactive, user-oriented model with ten commands. The user can edit parameters and driving variables, display process-response curves for all combinations of processes and driving variables, run a simulation for any length of time, print any or all state-variable results, debug loadings and rates during the simulation, tabulate the results, obtain line-printer and graphics-device plots, dump common block contents, and access an extensive HELP file.

The model is written in standard FORTRAN IV and will run in 22k on a PDP 11/03 with overlaying. It has also been tested on an IBM 3033. The program is well structured and is easy to understand. System-dependent features are restricted to two optional subroutines: one that handles operations such as file numbering and time calls and one that provides an interface to graphics terminals and plotters.

This Project Summary was developed by EPA's Environmental Research Laboratory, Athens, GA, to announce research 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

The PEST model has been under development for the past four years in response to the need for a detailed, chemically and biologically realistic model to predict the fate of toxic organic materials in natural aquatic environments. As such, its development has paralleled that of several other fate models; however, each model has its particular emphasis, and PEST fulfills a need for detail and biologic realism that is not addressed by other models.

PEST can be considered an evaluative model; it is intended to be used primarily to indicate the relative importance of the various processes under well-defined environmental conditions and to determine the environmental compatibility of particular organic materials. Many of the demands placed on the EPA relative to evaluating new materials can be answered through the expediency of such a process-oriented evaluative model. The model can also assist in the extrapolation of data from laboratory experiments and microcosms to natural environments.

PEST combines detailed chemical kinetics and bioenergetics to permit examination and evaluation of the behavior of toxic organic materials in the context of the entire aquatic ecosystem. Of course, use of such a complex model requires an understanding of the many assumptions and parameters, as well as a knowledge of the mechanics of the program. The purpose of this report is to acquaint the potential user with the details of PEST so that the model can be used both easily and wisely.

PEST is capable of simulating the time-varying concentration of a toxic organic material (TOM) in each of as many as 16 carrier compartments. The 16 state variables can be parameterized to represent a variety of TOM-carrier associations typical of aquatic ecosystems (for example, Figure 1).

The state-variable equations are ordinary differential equations with source and sink terms for the various processes that result in additions to, and losses from, the carriers. Broad categories include TOM in: plants, such as phytoplankton and macrophytes; animals, such as zooplankton, waterbugs, zoobenthos, and fish (different species and/or age classes); dissolved phase, either in the water column or in interstitial water; particulate organic matter, either suspended or as bottom sediment; floating organic matter, usually as a surface film; and clay, either suspended or as bottom sediment.

The source and sink terms for the state variables are represented by

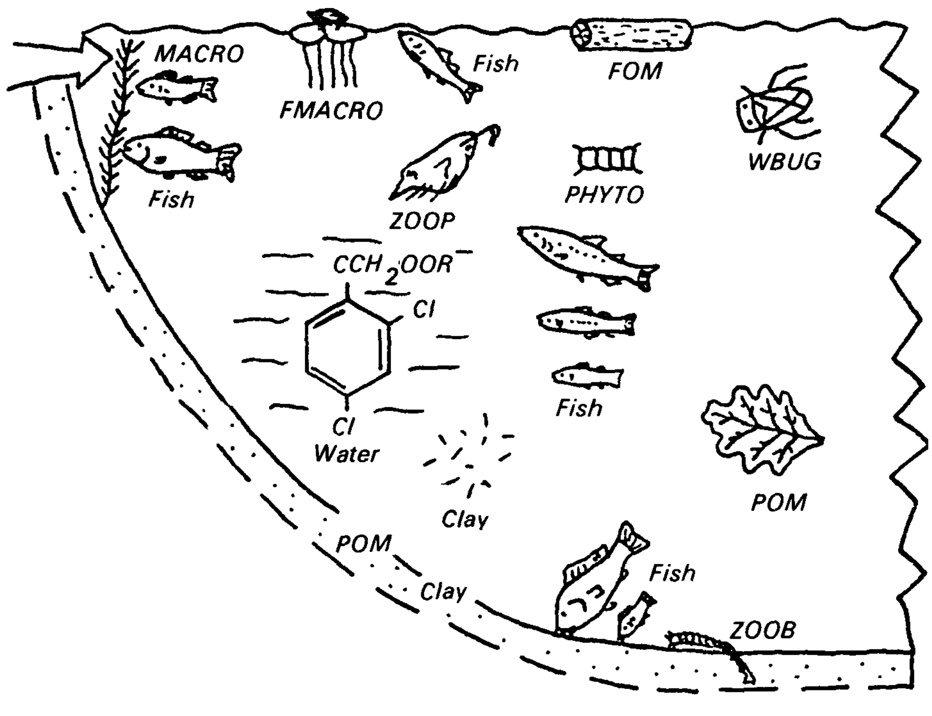

Figure 1. *Compartments in the PEST model. FMACRO = floating macrophyte, MACRO = macrophyte, FOM = floating organic matter, POM = particulate organic matter, WBUG = water bug, ZOOB = zoobenthos, ZOOP = zooplankton, PHYTO = phytoplankton.*

process equations. Most of the process equations are non-linear and involve several environmental factors (Figure 2).

Output from the model includes: (1) the time-varying concentration of the toxic material in each carrier (ppm), (2) the percent distribution of the toxic material among the carriers, and (3) the half lives of the toxic material in each carrier. One can also obtain plots of the degradation rates, both as they vary through time and as a function of environmental factors.

The model has been verified with process-level laboratory data for several compounds and with ecosystem data from fish ponds in Missouri and Israel and from a reservoir in Iowa. The site constants and environmental driving variables for these ecosystems constitute useful "prototype" data sets that enhance the value of the model for evaluative purposes.

Data Requirements

Data requirements depend on the intended use of the model. If PEST is to be used as an evaluative model, as originally intended, then default data on prototype sites (such as verification sites) may be sufficient to characterize the behavior and fate of a toxic organic material; therefore, site data would be unnecessary. If the model is to be applied as a diagnostic tool in order to better understand the fate of a compound at a particular site, then an accurate characterization of the site is required. If the problem involves bioconcentration in a particular group of organisms, then it will be necessary to accurately characterize the metabolic requirements and feeding preference of the organism.

Verification

The philosophy of verification was to use available parameter values, confirm the validity of the process equations by inspecting the process-response curves, and then apply the model to the particular site without calibration. If the fit to the observed data was not acceptable, the formulations were re-examined and improved, but the parameter values were not changed. This approach was taken because it was believed that there would not be opportunity or rationale for "fine-tuning" the parameter values in PEST

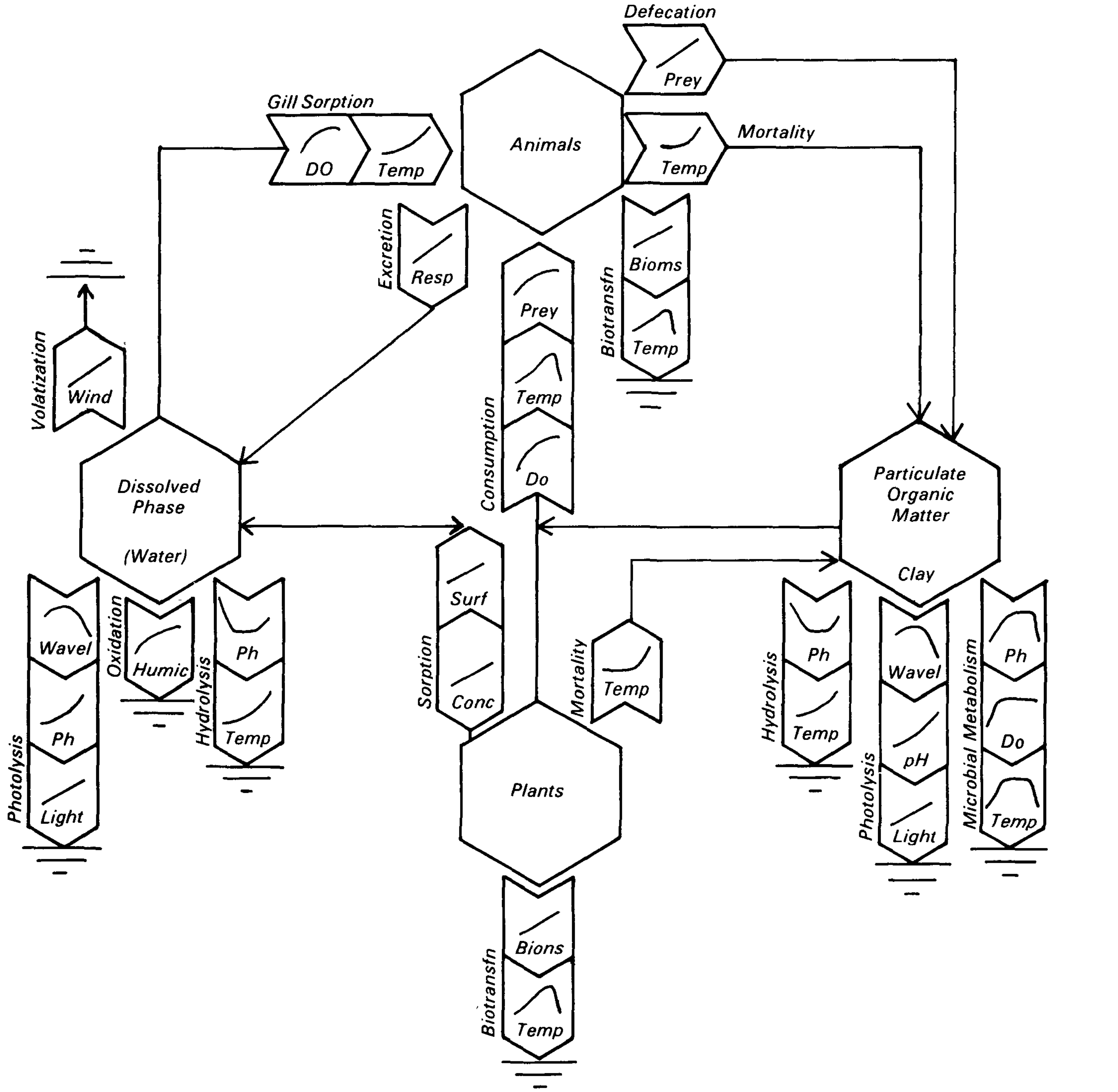

Figure 2. *PEST process flow chart.*

using observed data when PEST was used as an evaluative model for new compounds.

One of the verification sites was the Fish and Wildlife Service's National Fisheries Research Laboratory, Columbia, Missouri. Pentachlorophenol was introduced in 4 applications of 0.2, 0.2, 0.4, and 0.4 ppm in each of 3 low-nutrient ponds without macrophytes. The ponds were 297.28 square meters in area and had an average depth of 1.48 meters. Data were given for concentrations in water, bluegills, largemouth bass, and channel catfish. Even without calibration, PEST gave reasonable results in comparison with observed results.

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The complete report, entitled "Modeling the Fate of Toxic Organic Materials in Aquatic Environments," (Order No. PB 82-254 079; Cost: $16.50, subject to change) will be available only from:
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