Modelling Radionuclides and Pesticides in Food Chains*

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Abstract

Some aspects of modelling the kinetics of trace substances in food chains are discussed. The problems of sampling in space, time, and "systems" are considered in light of some case-histories and a food-chain simulation model.

This paper is largely a progress report and a discussion of some on-going work. It deals with our recent efforts to establish useful models of the behavior of a variety of contaminants in food-chains. It is predicated on the supposition that much of the present knowledge of the kinetics of radionuclides in food chains is directly applicable to a much wider range of substances, such as DDT and mercury. A major concern here is with what may be called "the sampling problem." That is, if it is assumed that the principles of first-order kinetics provide a reasonable mathematical model of the actual processes governing pollutants in food-chains, then what constitutes an efficient field sampling program? An earlier paper (Eberhardt and Nakatani, 1969) outlines the basic elements and philosophy of our current approach.

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The rationale of our recent efforts has these components: (1) to establish some "case histories" by examining a number of sets of actual field data, (2) to construct computer simulation models for individual case histories, (3) to investigate non-linear least-squares methods as tools for fitting models to data, (4) to attempt to elucidate some general principles that may be appropriate for predicting rate constants for substances and species that have not been directly studied, and, (5) to formulate questions about efficient sampling procedures. Given a "good" set of questions about sampling problems, and some potential strategies for sampling, a logical next step seems to be to build a computer simulation model that reflects what we know about some actual field situations, and to use the simulator to test the efficiency of various sampling programs. At present, it seems necessary to limit an approach via simulation to some rather simple situations, inasmuch as there are a number of unresolved questions about the systems of concern here. The complexity of a large-scale compartment model of a food chain is nicely illustrated by Kaye and Ball (1969:733).

The broad scope and complexity of existing and potential problems of environmental contamination is now widely appreciated and has been the subject of a great many committee reports and popular exposés. A recent detailed evaluation is available in the form of a report of the Study of Critical Environmental Problems (SCEP), titled "Man's Impact on the Global Environment" (M.I.T., 1970).

METHODS AND RESULTS

Models for food chains

A rather substantial number of recent reports demonstrate the applicability of first-order kinetic models to pollution problems. A few examples follow. J. Robinson (1967, 1969) has described an "ecosystem" model for chlorinated hydrocarbons and reviewed the evidence for postulating a first-order kinetic model for such substances. Kinetic models have been widely applied to radionuclides, as evidenced by the extensive review by Reichle, Dunaway, and Nelson (1970). A variety of exponential curves have been used to model uptake and retention of radionuclides in the interesting study of Hiyama and Shimizu (1969). R. A. Parker (1968) reported the application of similar models for simulating the role of dissolved nutrients in an aquatic system. Eberhardt, Meeks and Peterle (1970, 1971) applied kinetic models to simulation of the dynamics of radio-labelled DDT in a freshwater marsh. Eberhardt and Hanson (1969) devised a simulation model for an arctic food chain in order to follow kinetics of ^{137}Cs in the well-known lichen-caribou-Eskimo system. There is thus a fairly extensive literature showing applicability of first-order kinetic models to food chain phenomena.

Nearly all long-term studies (scale of years) seem to be characterized by pronounced seasonal cycles of the concentration of trace materials in biota. Such cycles, in combination with the pronounced variability usually observed in natural systems, lead to complications in fitting kinetic models to observational data. The investigator may then be forced to resort to uncertain postulates as to the nature of the system under study and to fit curves by "cut and try" methods.

In order to examine the difficulties of curve-fitting to models of relatively short-term studies, we have resorted to the model depicted in Figure 1. In this system a source releases a trace substance at an exponentially declining rate, and a fraction, c , is transferred to the first compartment (Y_1), which may be thought of as a plant. Two hypothetical animals are included, one having a single internal compartment and the other having two parallel-connected compartments, as shown in the diagram. Each compartment has an associated transfer coefficient and loss rate, as labelled. However, the parallel compartments are not cross-connected, as a consequence of the difficulty of ascertaining such internal transfer rates from observational data.

We have been testing non-linear least-squares computer fitting routines on data generated by a simulation model of Figure 1, using the following equations, and estimating the constants listed in each case:

Source

$$(1) Y_s = Ae^{-Bt} \quad (\text{routine estimates } A \text{ and } B)$$

"Plant"

$$(2) Y_p = \frac{CA}{B-\mu} [e^{-\mu t} - e^{-Bt}]$$

(routine estimates C , μ , or CA , B , and μ)

"one-compartment animal"

$$(3) Y_1 = \frac{C'A}{B-\mu} \left\{ \frac{1}{B-\tau} [e^{-Bt} - e^{-\tau t}] - \frac{1}{\mu-\tau} [e^{-\mu t} - e^{-\tau t}] \right\}$$

(routine estimates, C' and τ)

"two-compartment animal"

$$(4) \quad Y_2 = \sum_{i=1}^2 \frac{C_i A}{B - \mu} \left\{ \frac{1}{B - \gamma_i} [e^{-Bt} - e^{-\gamma_i t}] - \frac{1}{\mu - \gamma_i} [e^{-\mu t} - e^{-\gamma_i t}] \right\}$$

(routine estimates $\gamma_1, \gamma_2, C_1, C_2$)

An examination of the conditions and results of a number of field studies leads us to believe that inputs from a source (release of DDT, radiotracers, etc.) will most generally not be constant, and that the exponential decline may be the best approximation to actual conditions. It is thus necessary to deal with the rather complicated expressions above, and our experience thus far suggests that it will be essential to fit the resulting curves sequentially, starting with the source term and working progressively up the food chain.

We have not yet had enough experience with the system to judge how much random variation can be dealt with in fitting output data. The present simulator contains generators to produce random variables from a log-normal distribution at each stage. Each such generator depends on an adjustable common parameter (the coefficient of variation), so that variability in the entire system can be set at zero in order to test the various non-linear least-squares fitting schemes. Most of our initial experience has been with a "linearization" (or Taylor series) fitting method, but we are currently in final stages of changing to a version of a program developed by Marquardt, which combines the Taylor series and "steepest descent" methods (Cf., Draper and Smith, 1966, Chapter 10).

Even the preliminary efforts of building a simulator and checking out non-linear least-squares fitting routines are very useful in defining pertinent problems. A brief discussion of a few items follows.

Sampling in time

One of the immediate and more obvious conclusions to be drawn from testing the food-chain simulator described above is that a substantial number of observations is required to assure convergence to "reasonable" parameter estimates. The problem of sampling in time may thus be likened to a curve-fitting problem, wherein one might propose to investigate various "best" patterns of sampling points. However, the likelihood that most actual practice in field sampling must contend with the prospect of seasonal cycles in concentration may dictate evenly spaced sampling times as the conservative approach for initial surveys. Our attempt to model DDT concentrations (Eberhardt, Meeks and Peterle, 1970) suggests another difficulty, in that various species will have rather different uptake and retention curves, so that an optimum sampling pattern for one species may be very inefficient for most other species.

An interesting study of ^{89}Sr in a plant-rabbit food chain (Martin and Turner, 1966) illustrates the problem of balancing sampling in time against a need for sampling in space. The data presented by Martin and Turner indicate distinct differences among the more than 20 sites studied, but there are too few samples in time (4) to fit curves for each sampling location. There is thus a need for some

sort of joint analysis of the data which in turn requires advance decisions as to which parameters can reasonably be assumed invariant in space (or time?).

Differences in loss rates among representative species in the various trophic levels cause any time-dependent changes in concentration to show a lag effect as they pass up a food chain. This effect is apparent in the DDT study, and is particularly striking in arctic food chains, where it now seems that there may be distinct cycles at each trophic level (as has been reported by W. C. Hanson in another paper in this Symposium).

Sampling in space

One of the most difficult-seeming aspects of sampling in space is the prospect of feed-back effects, wherein part of the substance excreted (or otherwise lost) by some component of the biota may be "recycled." This problem is implicit in any approach to modelling that depends on a "conservation of mass" argument. In actual field experience, however, the mass of biota relative to that of other components of the environment is ordinarily very small. The usual situation, then, is that of a system with a very large "sink" (normally the substrate) and only a small fraction of the tracer substance is found in the biota at any point in time. Recycling or feed-back may thus largely constitute a second-order effect at most.

Any effort to assess a substance like DDT on a global scale cannot, however, exclude the prospect of feed-back effects. There is evidence of codistillation of DDT (Acree, Berova, and Bowman, 1963) and significant amounts have been detected in rainwater (Tarrant and Tatton, 1968). Understanding the ultimate status of DDT in the biosphere may

thus require a combination of a dynamic model and a balance study (Cf. the thousand-sample ocean baseline sampling program proposed in the SCEP report; M.I.T., 1970:176).

It thus seems that a crucial question for both modelling and judging environmental hazard is "how is the substance taken out of circulation, and at what rate?" An essential corollary is, "Can it return to circulation?"

Sampling the system

Our preliminary look at sampling problems suggests that time and space are inadequate coordinates for the purpose. There is a further need for "system-identification", more simply described as assessing the pathways of accumulation of a substance. This thus requires sampling species (or the biota in general) and calls for considerable experience and judgement not yet available for full efficiency in "systems analysis." If the pollutant is in fact doing serious damage to some species population, there evidently is a need to bring in another whole area of study -- population dynamics and dose-response phenomena. If several different substances are included in a study, it becomes apparent that there are indeed many dimensions involved.

CONCLUSIONS

Since this is largely a progress report, it is best concluded by suggesting some directions for future study. There is an urgent need for both material balance studies and for long-term studies. The balance studies are essential for pinning down the ultimate fate of various substances and thus helping to determine "safe" levels. Long-term studies seem essential as a precautionary device to help uncover the many unexpected effects influencing prediction about the future course of events. Another promising prospect is the introduction of a "pulse" of variously tagged or labelled substance at selected points in the system under study. One might thus hope to determine rates and pathways not otherwise accessible.

FIGURE LEGENDS

Figure 1. Sketch of a food-chain simulation model (Y_s = source, Y_p = plant, Y_1 = one-compartment animal, Y_2 = two-compartment animal. B , μ , γ represent loss rates, and the C_i , transfer coefficients).

Figure 1

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