The Use of the Analogue Computer in Pesticide Research

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The basic components of a general-purpose analogue computer are described in terms of their operational functions. Their use in pesticide research has been extremely limited but such examples as exist are reviewed.

Examples of the use of analogue computers are given. These include the simulation of single and consecutive first-order reactions, the sorption-desorption processes affecting the availability of pesticides in soils, diffusion and leaching in soils and the build-up of residues in soils following repeated annual applications to the soil surface.

1. Introduction

Analogue computers have rarely been used as aids to pesticide research, or indeed to any biologically-based research, perhaps because of the difficulty of describing the systems of interest in precise mathematical terms. However, the analogue computer is best considered as a device for the approximate simulation of physical systems, rather than as a particular type of calculating machine, and so its more extensive use in pesticide research might be expected. A valuable description of the analogue simulation of a number of typical processes occurring in chemistry and biology has been published by Röpke and Riemann.1

The main characteristic of the analogue computer is its ability to solve a series of simultaneous ordinary differential equations. The behaviour of these equations can be studied rapidly and conveniently and their response to changes in the various parameters can be measured with the greatest convenience.

A variety of analogue computers are available commercially, ranging from small desk-top machines to very large and expensive hybrid computers, which consist of an analogue computer containing 200 or more amplifiers interfaced with a digital computer. No attempt is made in this paper to discuss these large machines, which are to be considered as tools for the specialist. The examples discussed below can be handled by small to medium sized machines which can be programed and operated by most people following a minimum of tuition. Whilst most of these examples have simple analytical solutions they are used here to illustrate the operation of analogue computers.

1 Presented at a symposium The computer as an aid to pesticide research on 15 October 1973, organised by the Pesticides Group and the Physicochemical and Biophysical Panel, Society of Chemical Industry.
Many general analogue computer publications include a comparison of analogue and digital computers. This is omitted here in order to emphasise that the analogue computer is primarily a machine for constructing an electrical model of a physical system, rather than some sort of alternative to a digital computer.

2. The general-purpose analogue computer

General-purpose analogue computers consist basically of a modular arrangement of d.c. operational amplifiers and coefficient potentiometers together with an accurate source of reference voltage and a mode control and addressing system. Most medium and large-sized computers are fitted with a range of additional components which increase the flexibility of the computations. The inputs and outputs of each component are brought to terminals on a colour-coded patchboard and interconnections are made by multiple plugs and patch cords.

The basic component of the computer is the d.c. operational amplifier which may be considered as a "black box" capable of performing the unit operations of addition, multiplication and integration on input voltages. Modern operational amplifiers utilise solid state circuitry and their design and performance have been adequately described elsewhere. The input voltages, from a reference power supply, are scaled to represent problem variables and the output voltages may be monitored by a digital voltmeter, pen recorder or similar device. Potentiometers, or coefficient multipliers, permit voltages to be set to predetermined levels and act as constant multipliers. The generally agreed symbols for these units are shown in Table 1, together with the operations that they perform. In passing through an operational amplifier the sign of the voltage is reversed and care has to be taken to use one-input inverting amplifiers where necessary.

The majority of problems require that all parameters are scaled either for amplitude or for time. Amplitude scaling is governed by the size of the reference voltage, which is

<table>
<thead>
<tr>
<th>Component</th>
<th>Symbol</th>
<th>Operation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Potentiometer</td>
<td>$y = ax$</td>
<td>$0 \leq a \leq 1$</td>
</tr>
<tr>
<td>Summing amplifier</td>
<td>$y = -(s + t + u)$</td>
<td></td>
</tr>
<tr>
<td>Inverter</td>
<td>$y = -x$</td>
<td></td>
</tr>
<tr>
<td>Integrator</td>
<td>$y = -\int_0^t x , dt - c$</td>
<td></td>
</tr>
</tbody>
</table>
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normally $\pm 10$ or $\pm 100$ V. No output must exceed this value, but very small voltages should always be avoided if possible. Long periods of computation are also undesirable, but this depends upon the quality of the amplifier components. The ability of analogue computers to work at high speed is a distinct advantage but again care must be taken to ensure that the speed is not beyond the capacity of the slowest components, which will probably be relays operating switches. Scaling can be a prodigious task but the techniques are described in most textbooks at considerable length.

The accuracy of analogue computer solutions is almost impossible to define and may vary between 0.05 and 15%. This is because the accuracy depends on the particular problem, component errors being compounded in some cases and cancelled in others. The accuracy of individual computing elements can vary between 3 and 0.005% of full scale, but costs increase rapidly if accuracies of better than 0.2% are required.

2.1. Operation of analogue computers

One of the basic operations of the analogue computer, that of integration, may be illustrated by the solution of a first-order differential equation. Consider a typical hydrolytic reaction in which the rate of hydrolysis of a component $A$, initially at concentration $A_0$, is proportional to its concentration. This is described by the equation:

$$\frac{dA}{dt} = -kA$$

where $k$ is the rate constant.

If a voltage corresponding to $dA/dt$ is passed into an integrator the output will be equivalent to $-A$ and this is converted into $-kA$ by passing it through a coefficient potentiometer set to a value equivalent to the rate constant $k$. The output of the potentiometer ($-kA$) is equal to $dA/dt$ and so if this is connected to the input of the integrator the equation is satisfied. It then remains to incorporate the initial condition that when $t = 0$, $A = A_0$. The circuit diagram required is shown in Figure 1. If the output of the integrator is connected to a pen recorder the familiar exponential curve will be displayed. The effect of varying $k$ or $A_0$ may then be rapidly evaluated.

![Figure 1. Analogue computer circuit for a first-order reaction.](image)
by soil. If a soil (m g) is added to an aqueous solution of a pesticide (volume v, concentration C₀) we have, assuming that adsorption is completely reversible:

\[ C_s \xrightarrow{k_a} C_w \xleftarrow{k_d} C_s \]

where \( C_s \) = concentration of pesticide adsorbed by the soil particles,
\( C_w \) = concentration of pesticide in the soil water,
\( k_a \) = rate constant of adsorption,
\( k_d \) = rate constant of desorption,

and so:

\[ \frac{dC_s}{dt} = k_a C_w - k_d C_s. \quad (1) \]

The mass balance equation is:

\[ vC_o = mC_s + vC_w \]

and so:

\[ \frac{dC_w}{dt} = -\frac{m}{v} \frac{dC_s}{dt}. \quad (2) \]

Equations (1) and (2) may be solved on the analogue computer using the circuit diagram shown in Figure 2. The output of the integrators 1 and 2 may be plotted on an x–y recorder and would have the slopes shown diagrammatically in Figure 3.

![Circuit diagram](image)

**Figure 2.** Circuit to simulate the adsorption–desorption process.

Additional reactions and rate processes such as chemical or microbiological decomposition of the pesticide may be added to this basic adsorption–desorption model. Such a model also provides the basis for much of the work that has been done on the distribution of drugs between blood and body fat. However, as the number of equations increases so the number of computing elements must increase, since they all operate simultaneously.

### 2.2 The decomposition of trifenmorph in irrigation water

An example of the use of an analogue computer in solving equations related to a set of consecutive reactions is provided by the decomposition of the molluscicide "Frescon".*

* Shell registered trademark.
containing trifenmorph, 4-(triphenylmethyl)morpholine. This compound decomposes in aqueous solutions to triphenylmethanol (TPC) at a rate which depends on the pH. At concentrations of interest this dependence is adequately described by the empirical relationship:

\[
\log_{10} \text{(half-life)} = \text{pH} - 6.
\]

In laboratory determinations in buffer solutions at pH = 7.8 the half-life is 63 h, but at the same pH in irrigation canals in Egypt and the Sudan the half-life was found to be only 20–30 h. Inspection of the field analytical data showed that although the concentration of trifenmorph decreases more rapidly than in laboratory experiments the TPC concentration increases at the same rate in both the laboratory and field experiments. Furthermore, the sum of the two concentrations decreases to a minimum and then increases to the theoretical value.

These observations indicated that at least one and probably two other reactions were occurring in irrigation water and so the following model was suggested.

\[
\begin{align*}
\text{Trifenmorph} & \quad \xrightarrow{k_1} \quad \text{Triphenylmethanol} \\
& \quad \xrightarrow{k_2} \quad \text{R} \\
& \quad \xrightarrow{k_3} 
\end{align*}
\]

\(R\) is some unknown species, possibly an adsorption complex with suspended silt, \(k_1\) is the rate constant for hydrolysis which is determined by laboratory experiments and \(k_2\) and \(k_3\) are unknown rate constants.

The above model is described by the following equations:

\[
\begin{align*}
\frac{dF}{dt} &= -k_1 F - k_2 F \\
\frac{dR}{dt} &= k_2 F - k_3 F
\end{align*}
\]
\[
\frac{dT}{dt} = k_1 F + k_3 R
\]

where \( F \) = concentration of trifenmorph
\( T \) = concentration of triphenylmethanol
\( R \) = concentration of \( R \), the unknown species.

These equations may be solved on the analogue computer using the circuit diagram shown in Figure 4.

![Figure 4. Simulation of the decomposition of trifenmorph.](image)

![Figure 5. Comparison of calculated and observed concentrations in irrigation canals.](image)
The rate constant $k_1$ was known from laboratory data and it was possible to determine $k_2$ and $k_3$ by adjusting the respective potentiometers until the curves matched those determined by field analysis. The rate constant $k_3$ was in fact found to be almost equal to $k_1$. An example of the output of the various operational amplifiers is shown in Figure 5.

2.3. The application of trifenmorph to flowing water

Many devices are available to increase the versatility of the basic analogue computer. Most modern instruments are equipped with components which permit logical decisions to be made or constraints to be applied at appropriate times during the computation. One of these is the voltage comparator which is essentially a high-speed switch which changes its state when a sign-change occurs between an applied reference voltage and a varying voltage generated within the computation.

An example of the use of a number of comparators is in the simulation of the application of trifenmorph to flowing water. This compound can be added slowly, but continuously, at one point in an irrigation system upstream of the area to be treated. One particular irrigation system which has been treated in this way consists of a main feeder canal which transports water to a series of storage dams. These in turn feed small canals which lead into the fields to be irrigated. Water flows continuously into the dams but they supply water to the fields for only 10 h each day, Monday to Friday. No water is used on Saturday or Sunday and consequently the dams become recharged on these days.

This system was simulated on the analogue computer in an attempt to optimise the use of trifenmorph. The pattern of water use was simulated by means of comparators which caused the output velocities from the dams to be zero during 14/24th of the time designated on the computer as one day, also during 2/7th of the time designated as one week. This timing was done by generating two sine waves on the computer, one with a frequency of 1 cycle/“day” and the second with a frequency of 1/7th cycle/“day” and feeding these into the comparators. The circuit used for this problem is shown in Figure 6 and a typical output is shown in Figure 7.

3. The diffusion and leaching of pesticides in soils

The inhomogeneity of soils makes it very difficult to construct mathematical models of transport processes within them although a number of attempts have recently been made to do this. The equations of even relatively simple models are sometimes difficult to solve because they involve two independent variables, time and distance. This means that some approximation method must be used which reduces the partial differential equations to sets of ordinary differential equations.

3.1. Diffusion

Consider the diffusion of a pesticide from a cylinder of uniformly treated soil into an untreated cylinder of soil in contact with it. The variation of concentration ($C$) with
time \( t \) and the distance \( x \) in a cylinder of unit cross-sectional area is described by Fick's law of diffusion:

\[
\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2}
\]

where \( D \) is the apparent diffusion coefficient. The boundary conditions are that when \( t = 0, C = C_0 \) for \( x > 0 \) and \( C = 0 \) for \( x < 0 \).

The most generally accepted analogue computer approach to a partial differential equation such as this considers the solution \( C(x, t) \) only for a discreet set of values \( x = 0, Ax, 2Ax, \ldots, nAx \) of the space variable \( x \). Derivatives with respect to \( x \) are replaced by suitably chosen difference approximations. A first-order central-difference approximation to \( \partial^2 c/\partial x^2 \) in Fick's law yields:

\[
\frac{dC_i}{dt} = \frac{D}{Ax^2} (C_{i+1} - 2C_i + C_{i-1}).
\]

Figure 8 shows a suitable computer set up for the solution of this equation.

This simple computer set up is readily modified to account for various types of boundary conditions and even for variable diffusion coefficients. However, the difference approximation technique also presents serious difficulties. A sufficiently large set of differential difference equations may require a formidable number of computing elements and computer set-ups can be unstable or conditionally stable, so that noise
and component-error effects are greatly magnified. Errors associated with the finite-difference approximation require careful investigation.

A very considerable reduction in the required analogue computer capacity may be achieved if the partial differential equations are made discreet with respect to time rather than distance. To do this requires a storage memory, ideally a digital computer interfaced with the analogue computer. Discussion of the use of such hybrid computers is outside the scope of this paper.

3.2. Leaching

One approach to the leaching of pesticides in soils is based on the rate theory of chromatography developed by Lapidus and Amundson.11 Their general equation is the material balance over a thin layer of a chromatography column. If this is modified to account for chemical decomposition of the pesticide we have:

\[
\frac{\partial C_w}{\partial t} = D \frac{\partial^2 C_w}{\partial x^2} - \frac{1}{E} \frac{\partial S}{\partial t} - r \frac{\partial C_w}{\partial x} - kC_w
\]  

(3)

where \(C_w\) = concentration of pesticide in soil water (µg/ml),
\(S\) = concentration of adsorbed pesticide (µg/g),
\(E\) = fractional moisture content (ml/g dry soil),
\(r\) = velocity of water in the soil pores (cm/week),
\(x\) = soil depth, positive downwards (cm),
\(D\) = bulk average diffusion coefficient (cm² week⁻¹),
\(k\) = rate constant for decomposition (week⁻¹).

If the adsorption is represented as

\[C_w \xrightleftharpoons[k_a]{k_d} S\]

where \(k_a\) is the rate constant for adsorption and \(k_d\) the rate constant for desorption, then

\[
\frac{\partial S}{\partial t} = k_a C_w - k_d S.
\]

(4)
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Equations (3) and (4) describe the behaviour of the compound in the soil subject to the assumptions made in their derivation. These are that the adsorption is linear and completely reversible, i.e. $k_a$ and $k_d$ are constants; $D$ is independent of concentration and is constant; the velocity of the water in the soil is a constant; the soil does not shrink or swell and so $E$ is a constant. The assumption that the water velocity is constant gives most cause for concern if absolute estimates of leaching are required. However, when only comparative estimates are required objections to this assumption are minimised.

Before any attempt can be made to solve (3) and (4), initial and boundary conditions need to be specified. These can be varied widely depending on the nature of the input of the chemical into the soil. In general they may be described as

\[(a) \quad C_w(x = 0, t = 0) = 0\]
\[(b) \quad \left( \frac{\partial C_w}{\partial t} \right)_{x = 0} = \text{function of the mass of chemical applied to the soil surface.}\]

The combination of equations (3) and (4) is a third-order partial differential equation, which would be very difficult to solve. It has therefore been simplified by assuming that diffusion is small compared with mass flow (i.e. $D$ can be ignored) and also that adsorption equilibrium is attained rapidly (i.e. $k_d$ is large). We then have

$$\frac{\partial C_w}{\partial t} = \frac{1}{1 + K/E} r \left[ \frac{\partial C_w}{\partial x} - k C_w \right]. \quad (5)$$

where $K = k_a/k_d$.

The first-order partial differential equation may be solved by means of an analogue computer after transformation into a finite difference equation. This transformation is essentially equivalent to the introduction of the theoretical plate concept of chromatography, since it consists of dividing the column length into a number of equal parts of length $Ax$. The transformed equation which is solved on the computer is:

$$\frac{d(C_w)_n}{dt} = \frac{r}{Ax(1 + K/E)} [(C_w)_{n-1} - (C_w)_n] - \frac{k(C_w)_n}{(1 + K/E)} \quad (6)$$

where $(C_w)_n$ is the solution concentration within the theoretical plate number $n$ and $(C_w)_{n-1}$ that in the plate immediately above it. The circuit diagram for this is shown in Figure 9 and an example of the output of ten amplifiers is shown in Figure 10. In this diagram the concentration in each successive soil layer is plotted against time.

The number of theoretical plates that can be simulated is restricted by the number of integrators that are available on the computer. Thus on a small computer (e.g. 15 integrators) it may not be possible to simulate the height of an experimentally-determined elution curve, although the general shape and the position of maximum concentration would not be affected.

This simple model of the leaching process may readily be modified by altering the boundary conditions to study the effect of various types of controlled-release formulations. Studies of this nature have been reported in which an attempt was also made to
Figure 9. Circuit for the simulation of leaching without diffusion.

\[ a = \frac{r}{(1 + k/E)} \Delta x, \quad b = \frac{k}{(1 + k/E)} \]

Figure 10. Variation of pesticide concentration with time in a column of 10 equally thick sections of soil.

assess the effect of controlled-release formulations on the availability of a pesticide to a pest population.

3.3. Mode control

An essential component of the analogue computer is the mode control unit. On the simplest machines four operating modes are available, compute, hold, reset and potentiometer-set, and many also have a repetitive mode in which the computation is performed repeatedly for selected operating periods. These modes are usually selected by push-button controls but on more sophisticated machines the mode of each integrator may be selected automatically.
Figure 11. Distribution of a pesticide in a column of soil following annual additions of the pesticide to the soil surface. (Curves for even numbered soil layers only.)
A simple application of automatic mode control is for the study of the effect of repeated annual surface applications of a pesticide on the distribution of residues in the soil profile. The computer circuit for this could be similar to that in Figure 9 except that at the end of a period of time defined on the computer as 1 year, all of the integrators except the first would be switched into the "hold" mode. The first integrator would be reset to its initial value and the "compute" mode would then be selected. By continuing this sequence for a sufficiently long time the equilibrium levels of the pesticide residue could be determined. Figure 11 shows the output of the amplifiers of Figure 9 when operated in this way.

4. Conclusions

The analogue computer is a valuable instrument for investigating the general behaviour of many dynamic processes of interest in pesticide research. Its great advantage is its ease of operation and the excellent man–machine interaction that is possible.

It is a disadvantage that as the size of the problem increases the size of the computer must also increase. However, a medium-sized machine can deal with sufficiently large problems to be useful and can be helpful in exploring the behaviour of systems which might later be simulated by means of one of the many digital simulation languages that are now available. Although the accuracy of analogue computer solutions is not as high as that of those obtained from a digital computer it is usually better than that of the data which most experiments in pesticide research generate.

References