

MATHEMATICS OF STREAM AND ESTUARY PROBLEMS

by *J. V. Leeds, Jr.*

Introduction

A mathematical model of a stream or estuary is developed in this paper. The principles discussed in previous papers are utilized in the development. This paper is, in a sense, an extended example illustrating material previously covered. First, a very simple mathematical model is developed in order that the complexity of the model does not obliterate the assumptions made in obtaining the model. Next, certain analytical and computer solutions are obtained for this model which illustrate the usefulness of a mathematical model.

Background

Before developing the equations, i. e., the mathematical model, the problem itself must be put into perspective. The task to be accomplished is not the analysis of present conditions of a particular stream. No one will ask of a mathematical model: "What is happening in the stream today? What condition is the stream in today?" These questions are answered by going out today and sampling the stream. The task to be accomplished is to provide a means by which the answers to questions of the following type may be obtained: "If the waste load is increased, what will happen to the stream? Since a new waste source must be added to the stream, where and how should it be added so that its effect is minimized and the cost of treatment is minimized? If one has to make measurements of a stream, where and how should the measurements be made? If the quality of the effluent is improved, how much will the stream improve?" These are the types of questions which should be asked of a mathematical model. Furthermore, one does not have a model unless it can answer questions of this type with necessary accuracy.

Not only must the model provide answers to questions about the future, but the model must be such that the engineer can use it to tell

Editor's Note: Mr. Leeds is Assistant Professor of Electrical and Environmental Engineering at Rice University.

him how he can force nature to work for him. The engineer wants the model to tell him how to design treatment plants. He wants the model to tell him where and how he should take measurements to verify that certain conditions are existing in the stream. Note, however, that the model does not tell him how nature works. It merely tells him what his present understanding of nature is.

Another word of philosophy: The development and solution of a mathematical model by necessity requires one to join with the mathematician. There is no point in claiming that the solution must exist because the real world behaves in such a manner. The mathematical model is not the real world. Thus, the work must be mathematically correct.

Furthermore, once the assumptions are made, everything else follows deductively from the assumptions. Therefore, in fitting the model to the real world, one must really fit the assumptions to the real world. Essentially, one is looking for a mathematical model which will approximate the real world.

In addition, one should realize that the material presented represents current knowledge. As a result of subsequent research and experience (and perhaps luck), these inadequate results will be improved upon. One should understand that the material presented here is subject to controversy. As discussed in the modeling paper, one must fit the mathematical model to the real world and furthermore, one must be capable of verifying the model and obtaining the constants in the model. In the area of stream and estuary analysis, there is a divergence of opinion of how to develop the simple model of the estuary.¹ The disagreement arises because the general equations are too complicated for present machines to solve. The view presented here is the one which will be perhaps the predominate one in the future.

Basically, one wants to know how a pollutant is distributed in a stream. The pollutant is mass. Thus, one requires that in any section of the stream, mass is conserved. One means by this statement that one can add the mass that has entered the section to the mass that was there, then subtract the mass that has left the section, and the resultant mass is the amount of mass presently in the section. Now this simple equation (and it is an equation) can become very complicated, and the solution may be very difficult, even on a computer. However, this is the basic conservation of mass equation.

Now in order to compute the mass that has entered the section one may have to write an additional equation. This equation is really a generalization of Newton's Law, which states that if you accelerate a mass, then that mass "experiences" a force proportional to the acceleration and to its mass. From this, one can develop the principle of con-

ervation of momentum. Again, this may be very difficult to write and solve, but it follows from the simple statement that force is proportional to mass times acceleration.

Last, in order to track certain changes that substances are undergoing and perhaps to compute the mass that has entered the section, one may have to write an additional equation. This states that the energy added to the system minus the energy lost from the system plus the energy originally in the system must equal the total energy in the system. (This follows from the first law of thermodynamics.)

Development Of A Simple Model

In this model, only the conservation of mass law will be used. The reason for this will develop later. Consider the simplest case: a stream of constant cross sectional area A with a constant velocity V . See Figure 1. Suppose that a substance is present whose distribution is to be calculated along the stream and in time. Furthermore, make the simple

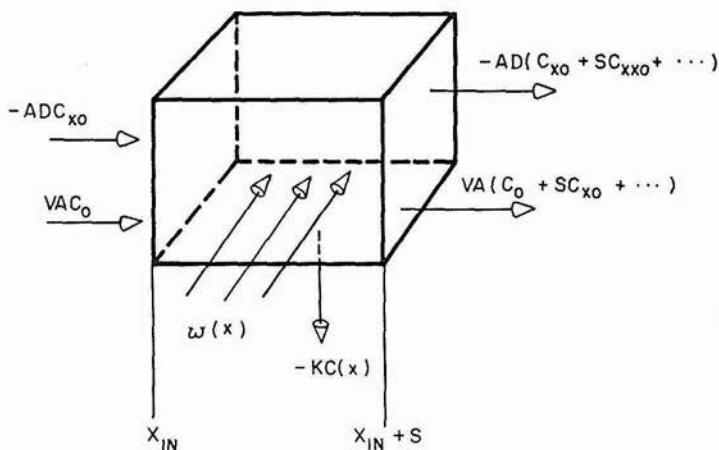


FIGURE 1 - BASIC STREAM

assumption that if the substance was kept in a bottle, the amount of the substance would decrease with time. In addition, suppose that the substance will diffuse throughout the volume if there is more in one part of the volume than in the other. Finally, the stream will bring new material into any fixed portion of the stream, and there is a source of the substance distributed along the stream. At any instant, all of this is occurring simultaneously. The problem is to write an equation which when solved will tell how the substance is distributed in time and space.

Note carefully that several assumptions have been made which cannot happen in the real world. It is extremely important in considering

any mathematical model that one examines the assumptions used to develop the model. Normally, everything is deduced logically from these assumptions. If these assumptions fit the physical world well, then the model will fit the real world well. However, these assumptions are usually given only slight emphasis in a development. Sometimes the assumptions are not given and must be inferred from the text. The set of assumptions is the most important part of any model.

The model could now be developed by writing the equation of continuity and using Fick's law to write the diffusion term. This was discussed in the transport section. However, here the development will be presented in its simplest terms and in detail so that one may clearly see the steps leading to the final equation.

Consider first the problem of disappearance of the substance. One certainly needs an expression which says that no more will disappear when there is no more left. In other words, the rate of disappearance is zero when none of the substance is present. Furthermore, one would expect that this rate must in some manner depend on the amount of the substance present, i. e., more mass would disappear in one second if ten pounds were present than if one pound were present. Denote that rate by R . Let the mass of the substance be denoted by M . Then examine an equation of the following form:

$$R = Mk(M) \quad (1)$$

Certainly, the rate is zero when M is zero. Furthermore, the rate depends on M . Now as discussed in the kinetics paper, the major problem is discovering what $k(M)$ is. Assume that $k(M)$ is a constant independent of M :

$$R = kM \quad (2)$$

Note carefully that no assumption is made about how much M was present but an assumption is made about the *rate* of disappearance of M . If one is successful in writing an equation, one is going to have an equation involving rates. Thus, since rate is a derivative, equation (2) becomes:

$$\frac{dM}{dt} = -kM. \quad (3)$$

Now there are two types of equations involving rates: ordinary and partial differential equations. Ordinary differential equations arise where one has only *one* dependent variable, e. g. time. Partial differential equations arise when one has more than one variable, e. g. space and time. In a river, one is concerned with both distance along the river and the particular time. Hence, the final equations will be partial differential equations.

Now consider a volume v . See Figure 1. The volume has length L .

Define a new term, C . This term is the density of a component, although it is normally called concentration. In a volume in which the mass is distributed uniformly, the total mass is the volume times the concentration. However, if the concentration is not uniform, one can still define an average concentration by dividing M by v . Then as we consider smaller and smaller volumes (i. e., proceed to the limit as v shrinks to zero) we see that we can define concentration by:

$$\int_v C \, dv = M \tag{4}$$

(Note that this does not agree with the physical world. As the volume shrinks, it eventually becomes smaller than one molecule. This is a useful approximation, however.)

Now consider the rate expression. The variable, C , is a function of both position and time, i. e., C equals $C(x, t)$. However, the mass in any particular volume v at a particular time t is certainly equal to:

$$M(t) = \int_v C \, dv \tag{5}$$

Putting this into the rate equation:

$$\frac{d(M)}{dt} = \frac{d}{dt} \left(\int_v C \, dv \right) = -k(M) = -k \left(\int_v C \, dv \right) \tag{6}$$

Since v is not a function of time, v is finite, and k is not a function of position:

$$\frac{d}{dt} \left(\int_v C \, dv \right) = \int_v \frac{dC}{dt} \, dv = -k \int_v C \, dv, \text{ OR } \int_v \left[\frac{dC}{dt} + kC \right] \, dv = 0 \tag{7}$$

Now if this is to hold for all values of t, x , then:

$$\frac{dC}{dt} = -kC \tag{8}$$

at each point, x, t . This is the final form of the rate equation. It says that the time rate of change of concentration due to a disappearance of a substance at any point in space and time is equal to a constant times the density at that point.

Now consider the model of the stream. See Figure 1. The control volume v has mass transported into it by the movement of the stream V . The rate that mass enters is equal to the velocity times the area times the density. Note that this is nothing more than saying “ q ” equals velocity times area, and the mass rate is q times the density.

Thus for x equal to X_{IN} , we have

$$q_{IN} = VA \quad (9)$$

$$\left. \frac{dM}{dt} \right|_{IN} = q_{IN} \cdot C_{IN} \quad (10)$$

Now at the other end, i. e., X_{OUT} q is the same:

$$q_{OUT} = VA \quad (11)$$

However, the density is assumed to be different, i. e., the density is assumed to be C_{OUT} . Thus

$$\left. \frac{dM}{dt} \right|_{OUT} = q_{OUT} \cdot C_{OUT} \quad (12)$$

Next consider the last expression for mass movement. Assume Fick's Law to hold. This states that in a solution where the concentration is a function of distance, that mass is transferred at a rate proportional to the rate of change of concentration with distance:

$$\frac{dM}{dt} = -AD \frac{\partial C}{\partial X} \quad (13)$$

Now digress for a moment. The function $C(x, t)$ is assumed to have the necessary properties so that it can be approximated by Taylor's series:

$$C(x, t) = C(x_{IN}, t) + (x - x_{IN}) \left. \frac{\partial C}{\partial X} \right|_{x_{IN}} + \frac{(x - x_{IN})^2}{2!} \left. \frac{\partial^2 C}{\partial X^2} \right|_{x_{IN}} + \dots \quad (14)$$

Thus, C_{OUT} is equal to:

$$C_{OUT} = C_{IN} + L \left. \frac{\partial C}{\partial X} \right|_{x_{IN}} + \dots \text{ where } x_{OUT} - x_{IN} = L \quad (15)$$

Next, define a shorthand notation for $C(x, t)$:

$$\frac{\partial^n C}{\partial X^n} = C_{\underbrace{XX \dots X}_n}, \quad \frac{\partial C}{\partial t} = C_t \quad (16), (17)$$

$$\left. \frac{\partial^n C}{\partial X^n} \right|_{x_{IN}} = C_{\underbrace{X \dots X}_n}_{x_{IN}} \quad (18)$$

Define: $x = X_{IN} + s$

$$\text{then: } C(x, t) = C_0 + SC_{x_0} + \frac{S^2}{2!} C_{xx_0} + \dots \quad (19)$$

$$\text{and } C_x(x, t) = C_{x_0} + SC_{xx_0} + \dots \quad (20)$$

$$C_t(x, t) = C_{t_0} + SC_{xt_0} + \dots \quad (21)$$

Next, the conservation of mass equation will be written.

Now, examine the control volume of Figure 2. In this volume mass

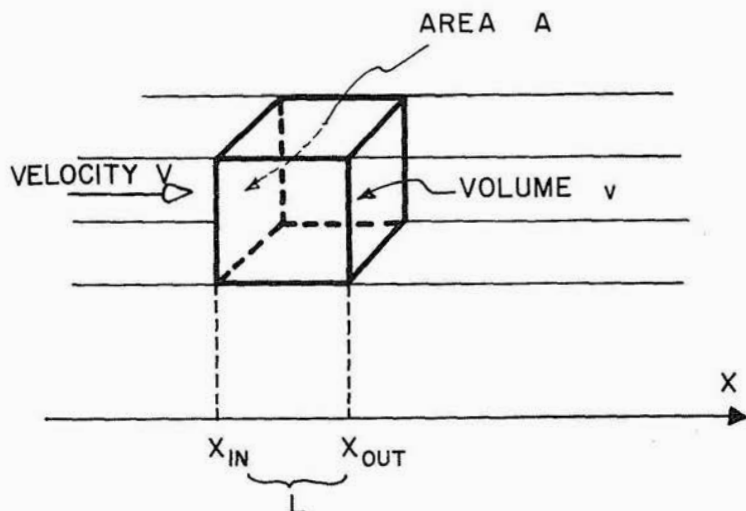


FIGURE 2 - CONTROL VOLUME

is conserved. Thus at X_{IN} , mass enters the volumes at these rates:

by diffusion: $- ADC_{x_0}$ (22)

by flow: $VAC_o x$ (23)

by a source term: $\int_{X_{IN}}^S W(x,t)dx$ (24)

Mass leaves the volume at $X_{IN} + S$ at these rates:

by diffusion: $- AD(C_{x_0} + SC_{xx_0} + \dots)$ (25)

by flow: $VA(C_o + SC_{x_0} + \dots)$ (26)

Mass disappears at a rate of:

$$\int_{X_{IN}}^{X_{IN}+S} AKC(x,t) dx = AK \int_0^S [C_o + SC_{x_0} + \dots] ds$$

$$= KAC_oS + KA \frac{S^2}{2} C_{x_0} + \dots$$
 (27)

Now the source term also has a Taylor series expansion:

$$W(x,t) = W_0 + W_{x_0} S + \dots \quad (28)$$

The amount that enters the volume is:

$$\int_{x_{in}}^{x_{in}+s} AW(x,t)dx = AW_0S + \frac{AS^2}{2} W_{x_0} + \dots \quad (29)$$

Finally perform the following operation:

$$\begin{aligned} \int_{t_0}^{t_0+\tau} (\text{Rate Mass Enters} - \text{Rate Mass Leaves} - \text{Rate Mass Disappears}) dt \\ = \int_{t_0}^{t_0+\tau} (\text{Rate Mass Changes}) dt \end{aligned} \quad (30)$$

This merely says that mass is conserved, i. e., the mass that has entered minus the mass that has left is equal to the mass that has accumulated in the interval of time τ .

The first integrand is:

$$\begin{aligned} -ADC_{x_0} + VAC_0 + AD[C_{x_0} + SC_{xx_0} + \dots] - VA[C_0 + C_{x_0} S + \dots] \\ + AS[W_0 + \frac{1}{2}W_{x_0} S + \dots] - KAS[C_0 + \frac{C_{x_0}}{2} S + \dots] \\ ADS[C_{xx_0} + \text{HOT}] - VAS[C_{x_0} + \text{HOT}] - KAS[C_0 + \text{HOT}] \\ + AS[W_0 + \text{HOT}] \end{aligned} \quad (31)$$

where HOT denotes terms containing s as a factor. Consequently as s goes to 0, these terms go to zero.

The rate that the mass is changing is:

$$\begin{aligned} A \int_{x_{IN}}^{x_{IN}+s} C_t dx = A \int_0^s (C_{t_0} + SC_{tx_0} + \dots) ds \\ = AS(C_{t_0} + \frac{S}{2} C_{tx_0} + \dots) \end{aligned} \quad (32)$$

Therefore, the complete expression (30) becomes:

$$\int_t^{t+\tau} \left\{ ADS[C_{xx_0} + \text{HOT}] - VAS[C_{x_0} + \text{HOT}] - KAS[C_0 + \text{HOT}] + AS[W_0 + \text{HOT}] \right\} dt$$

$$= \int_t^{t+\tau} AS \left[C_{t_0} + \frac{S}{2} C_{t_{x_0}} + \dots \right] dt \tag{33}$$

Now, if this is to hold for all values of t, then:

$$AS \left\{ D(C_{xx_0} + HOT) - V(C_{x_0} + HOT) - K(C_0 + HOT) + (W_0 + HOT) - (C_{t_0} + HOT) \right\} \equiv 0 \tag{34}$$

Since $AS \neq 0$, the bracketed term is identically equal to zero. Now take the limit of the bracketed term as S approaches 0. All HOT go to zero and:

$$\lim_{S \rightarrow 0} \left\{ D(C_{xx_0} + HOT) - V(C_{x_0} + HOT) - K(C_0 + HOT) + (W_0 + HOT) - (C_{t_0} + HOT) \right\} = DC_{xx_0} - VC_{x_0} - KC_0 + W_0 - C_{t_0} = 0 \tag{35}$$

Thus one arrives at the following partial differential equation (since X_{in} was arbitrary):

$$DC_{xx} - VC_x - KC + W_0 = C_t \tag{36}$$

Now what assumptions were made in deriving equation (36)?

- 1) D, V, K are constants.
- 2) D, V, K do describe *adequately* the physical processes.
- 3) C(x, t), W(x, t) can be expanded in a Taylor's series in x^2
- 4) The physical system is one dimensional (in space).
- 5) The substance "C" does not affect V.
- 6) No other substance affects the solution.
- 7) The system is linear. (D, V, K do not depend on C.)

(Note: The additional assumption is made that D is a diffusion term, not necessarily a molecular or an eddy diffusivity. The assumption is that mass diffuses into the section with D being a constant of proportionality.)

Verification

Now an equation has been derived and the assumptions upon which the equation is based have been listed. The deductive process flowing from the assumptions to the equation is clearly evident. Now another problem presents itself: does this mathematical model (i. e., equation [36]) approximate the real world closely enough?

Unfortunately, there is no general procedure to verify a mathematical model. There are some general principles. First, one must obtain estimates of parameters. Then, one must probe the model and probe the real world to see if they agree. One must make the probing independent of the

measurement of parameters. Otherwise, one is just curve fitting.

In this area, the model is of great help. First, it tells you what you have to measure. Second, if your measurements disagree with some of the assumptions, you must modify the model, (for example, k might depend on C). Third, the model and other mathematical considerations may dictate the kind of measurements and even the measurement procedure.

A specific set of measurements to obtain D , V , and K is given below. This is intended to be a simple set and to indicate the problems. It is not a detailed prescription to obtain the correct results. First, K could be obtained by taking samples of the water containing some of the substance and measuring the disappearance rate in the laboratory. Next, V could be obtained from velocity measurements of the river and an area measurement. But a river does not usually have a uniform cross section. So, one might expect variations in V as a function of X . Suppose an average is used:

$$V = \frac{1}{L^*} \int_0^{L^*} V(x) dx \quad (37)$$

However, $V(x)$ will be obtained not as a continuous function, but as a sampled function. One must evaluate the integral by using a difference approximation to $V(x)$. However, the experimenter is at liberty to choose the points x . Hence, one should use a high accuracy quadrature formula to obtain the integral. Thus, the model equation has dictated the experimental procedure.

Next, one might inject a dye into the stream, solve the equation, and match up the results from physical measurements and the model. This will determine D . Again, one has to decide where to measure. Again, an analysis of the model will indicate where. One must perform a sensitivity analysis and find the points where D affects the answer the most.

Having obtained D , V , K , one must now *independently* check the model. One must probe the model and the world. First, a model is usually easier to disprove than to prove. Thus, the tests should be set up so that some critical questions are asked of the model and the world. These usually come from analysis of the model. For example, one can calculate what kind of a distribution a source of C injected at $x=0$ and being a specified function of time will produce. Next, one can test whether or not the equations will give the right answers when another source at $x \neq 0$ is added. One can calculate the result and compare it with what happens. Note these calculations are *independent* of measurements of D , V , K . Next, one can perform a sensitivity analysis on D , V , K . If the accuracy with which one knows D , V , K will not bring the model into agreement with the test data, one needs to *change the model*.

General Equations

One can derive a similar equation in three space dimensions and time. It would serve no useful purpose to do this here. The interested reader is referred to the transport paper and to the reference listed in the notes.³

Solutions

One can for very simple situations obtain analytic solutions (even closed solutions) to equation (36). However, the evaluation of these solutions can be difficult. As an example, consider a river of infinite extent with the following conditions imposed:

a) $C(\pm \infty, t) \equiv 0$ (38)

b) $W(x,t) = \begin{cases} 0 & |x| > b \\ W_0 & |x| \leq b \end{cases}$ (39)

c) Steady state response only: $C_t = 0$ (40)

Now define some new parameters:

d) $\Gamma = A \sqrt{KDC/W}$ (41)

e) f) $\alpha = x\sqrt{K/D}$, $\alpha_0 = b\sqrt{K/D}$ (42), (43)

g) $N = V/\sqrt{K/D}$ (44)

h) $f(\alpha) = W(x,t)\sqrt{D/K} \int_{-b}^{+b} W(x,t) dx = \frac{1}{2}\sqrt{D/K} / b = \frac{1}{2\alpha_0}$ (45)

Then, the solution is:

a) $\Gamma(\alpha) = \frac{\frac{N + \sqrt{N^2 + 4}}{2} \alpha}{\alpha_0 \sqrt{N^2 + 4} (N + \sqrt{N^2 + 4})} \sinh \frac{N + \sqrt{N^2 + 4}}{2}$ (46)
 For $\alpha < -\alpha_0$

$\Gamma(\alpha) = e^{\frac{\frac{N + \sqrt{N^2 + 4}}{2} (\alpha - \alpha_0)}{\alpha_0 \sqrt{N^2 + 4}} - 1}$

b) $+ \frac{e^{\frac{\frac{N - \sqrt{N^2 + 4}}{2} (\alpha - \alpha_0)}{\alpha_0 \sqrt{N^2 + 4} (N - \sqrt{N^2 + 4})}}}{\alpha_0 \sqrt{N^2 + 4} (N - \sqrt{N^2 + 4})}$ (47)
 For $-\alpha_0 < \alpha < \alpha_0$

$$c) \quad \Gamma(\alpha) = \frac{2e}{\alpha_0 \sqrt{N^2 + 4} (N - \sqrt{N^2 + 4})} \sinh \frac{N - \sqrt{N^2 + 4}}{2} \alpha_0 \quad (48)$$

For $\alpha_0 < \alpha$

The details may be found in O'Connor and Lawler's paper.⁴

Now, the purpose in giving this solution is to show that for this very simple problem, the analytic solution is of almost no use. It would normally be evaluated on a computer. Thus having to resort to computer solutions for more complicated models is no great loss.

Now consider a computer solution. Suppose one has a river of finite extent and wishes to study three effects: 1) Since one must sectionalize to solve the equation, what is the minimum number of sections necessary for a satisfactory solution? (Obviously the cost, effort, and difficulty go up as the number of sections increases). 2) What is the effect of approximating this finite river by an infinite one? Phrased another way, how long does a river have to be before it can be considered infinite? 3) Suppose one must make a set of measurements to determine D? What accuracy should be maintained throughout the length of the river? How much variation is allowable in K, V and D before they can no longer be considered constants? In other words, what influence at a point X_0 , does an error in measuring D at X_0 plus b where b does not equal to zero have on the solution?

Note that each of these questions is asked before field work commences. The first evaluates the computer work required to do the problem. The second evaluates the correctness of the models as applied to the problem and indicates the region of the river of interest. The third actually determines what field procedures are to be followed in measuring parameters and evaluates the correctness of the model. This clearly shows the usefulness of a mathematical model.

Obviously, if this type of work is to guide field work it must be done before any field work of a great amount is accomplished.

Consequently, the data used to obtain a first estimate (in this case the values of D, K, and V) are likely to be in error. As the field work progresses, the model may be used to update the answers to these and other questions.

Now, consider Figure 3.⁵ Figure 3 shows the effect of changing the number of sections in the solution of the partial differential equation as a plot of the concentration as a function of distance at a particular time. The time is 25 days after a step change in source. It can be seen that the maximum error occurs roughly 2.1 miles upstream from the point of injection and that this error is approximately 3 per cent of the

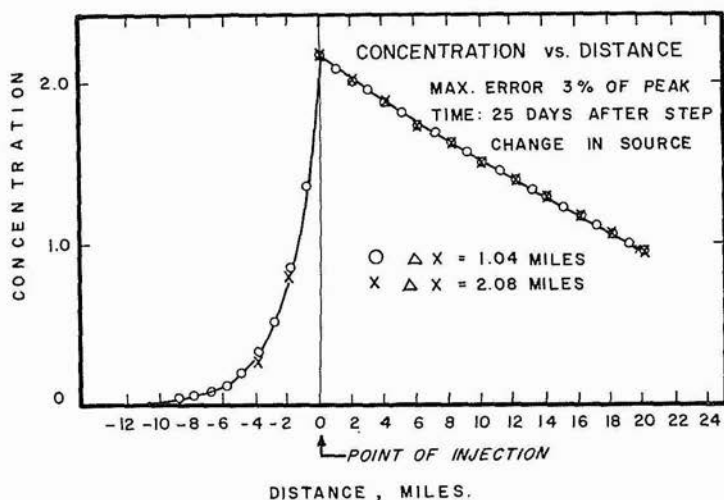


FIGURE 3- EFFECT OF SECTIONING

peak value of the concentration. Thus, a spacing of 5,500 feet per section is not required and a spacing of at least 11,000 feet per section may be used. It may be that after further investigation one could use even larger spacings to describe adequately the solution to this problem.

Now that the length of the section has been set as 11,000 feet, one may then examine the effect of length on the solution. Thus Figure 4 shows that a river which is 102 miles long can be considered essentially infinite for the magnitude of x less than 50 miles. One that is 27 miles

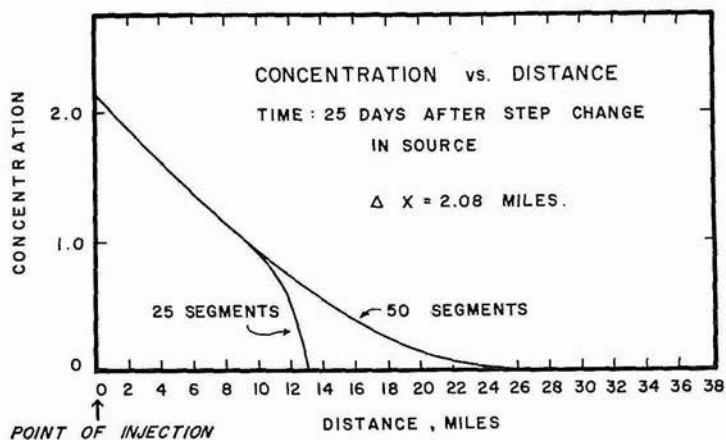


FIGURE 4- EFFECT OF LENGTH

long can be considered essentially infinite if one restricts oneself to a range of x less than 21 miles.

Now examine the effect of changing a parameter on the solution. This is done by calculating the relative sensitivity as a function of distance at a particular time step as shown in Figure 5. Presuppose that at 13 miles the parameter D , the diffusion coefficient, is changed and ask: what is the change in the solution? This is shown in Figure 5. If one multiplies the fractional change by the coefficient given in Figure 5 and then adds this to the value of the concentration at the particular point of interest,

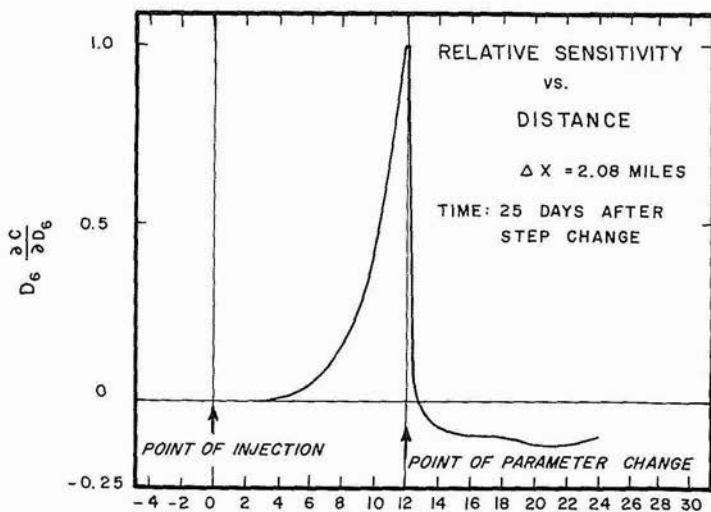


FIGURE 5 - EFFECT OF PARAMETERS

one can get the effect of changing the coefficient. Notice that the coefficient has most influence at the point where the parameter was changed. At the injection point, the effect has dropped to a negligible amount. In addition, notice that if the diffusion coefficient is increased, the concentration downstream decreases since more material is going upstream.

It might be worthwhile to give some indication of the cost of obtaining this data. The data presented represents two runs on the IBM 7094 computer. The problem was sectionalized so that 50 differential equations were obtained. Approximately 1,000 time steps were evaluated. This represents a total cost of approximately \$52.00 or seven minutes of computer time.

Conclusions

A mathematical model of a stream or estuary has been developed in this paper. The model itself is highly simplified. Each assumption which

has been made has been listed and discussed. An example of the use of the model to outline field procedures has been given. It shows, for example, that accuracy requirements on the measurement of the diffusion coefficient can be obtained quite easily.

NOTES

1. *Effects of Polluting Discharges on the Thames Estuary* (London: Her Majesty's Stationary Office, 1964), and D. J. O'Connor and J. P. Lawler, "Mathematical Analysis of Estuarine Pollution," presented at 55th National Meeting, AIChE, Houston, Texas (February 7-11, 1965).
2. This restriction on $C(x,t)$, $W(x,t)$ can be weakened considerably.
3. R. Byron Bird, Warren E. Stewart, and Edwin N. Lightfoot, *Transport Phenomena* (New York, 1960).
4. O'Connor and Lawler, op. cit.
5. The author wishes to acknowledge the help of one of his students, Mr. Hal Bybee, who provided the computer runs used to generate Figures 3, 4, and 5. The computer work was supported by a National Institute of Health Grant, FR-254-01, at the Common Research Computer Facility, Texas Medical Center, Houston, Texas.